CP4604

Queen Mary and Westfield College

UNIVERSITY OF LONDON

MSci EXAMINATION

REMOTE SENSING OF ATOMIC
AND MOLECULAR SPECIES PHY-914

18 MAY 1998 14:30

Time Allowed: THREE HOURS

Answer **THREE** questions only. No credit will be given for attempting a further question.

Each question carries 20 marks. The mark *provisionally allocated* to each section is indicated in the margin.

FORMULA:

$$\sum_{n=0}^{\infty} \exp^{-nx} = [1 - \exp^{-x}]^{-1}$$ where n is integer

DATA:

Intensity of black body radiation (power/unit area/unit solid angle/unit frequency):

$$B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{(\exp^{h\nu/k_B T} - 1)}$$

Planck's constant	:	$h = 6.63 \times 10^{-34}$	J s
Speed of light	:	$c = 3.00 \times 10^{8}$	m s^{-1}
Boltzmann's constant	:	$k_B = 1.38 \times 10^{-23}$	J K^{-1}

TURN OVER WHEN INSTRUCTED

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1. Define the *m*th moment, with respect to a given direction, of the specific intensity I_ν of radiation. [2 marks]

Show that the pressure p of radiation exerted on an arbitrary surface in a radiation field is related to the second moment K_ν of the field by

$$p = \frac{4\pi}{c}\int K_\nu d\nu . \qquad [6 \text{ marks}]$$

Consider two levels of a quantum system with energies ε_i and ε_j, where $\varepsilon_j > \varepsilon_i$. Define the Einstein coefficients A_{ij}, B_{ji} and B_{ij} terms of the population-densities n_i and n_j of the levels and the transition rates between them. [4 marks]

By considering the absorption of the radiation of all frequencies passing though a small volume of material, show that the absorption coefficient $\kappa(\nu)$, in the spectral line produced by transitions between these two levels, is related to the Einstein coefficients by

$$\kappa(\nu) = h\nu_o \left[n_i B_{ij} - n_j B_{ji}\right]\phi(\nu),$$

where $\phi(\nu)$ is the line profile, normalised so that,

$$\int_{\text{line}} \phi(\nu) d\nu = 1,$$

and

$$h\nu_o = \varepsilon_j - \varepsilon_i . \qquad [8 \text{ marks}]$$

2. The orbital, spin and total angular momenta of a single electron in an atom are given respectively by:

$$[l(l+1)]^{1/2}\frac{h}{2\pi} \qquad [s(s+1)]^{1/2}\frac{h}{2\pi} \qquad [j(j+1)]^{1/2}\frac{h}{2\pi}$$

where h is Planck's constant and l, s and j are the respective quantum numbers. Describe the Russell-Saunders approximation for coupling the orbital and spin angular momenta in poly-electronic atoms. Your description should outline the procedures and rules used when atoms with equivalent and non-equivalent electrons are considered. [8 Marks]

Explain the meaning of *configuration*, *term*, and *spectroscopic state* as used in atomic spectroscopy. [4 Marks]

For an atom with non-equivalent electrons in a 3d3p configuration use *ls* coupling to determine:

a. The resultant total orbital angular momentum ***L***
b. The total spin angular momentum ***S***
c. The overall angular momentum ***J*** [6 Marks]

and thus determine the possible spectroscopic states for this atom. Your answer should use and explain the correct spectroscopic notation. [2 Marks]

3. For a system of N molecules in equilibrium, the Boltzmann population N_i of energy level E_i is given by

$$N_i = \frac{N d_i}{Q(T)} \exp\left(-\frac{E_i}{kT}\right)$$

where d_i the degeneracy, T the absolute temperature, k the Boltzmann constant and $Q(T)$ is the partition function given by,

$$Q(T) = \sum_{n=0}^{\infty} d_n \exp\left(-\frac{E_n}{kT}\right)$$

Assuming the vibrational states of a diatomic molecule are all nondegenerate, with vibrational energies approximated by,

$$E(v) = \frac{h}{2\pi}\omega\left(v + \frac{1}{2}\right) (v = 0, 1, 2, \ldots),$$

where ω is the angular frequency, show that the number of molecules in state v can be written as:

$$N_v = \frac{N}{Q(T)_{vib}} \exp\left(-\frac{h}{2\pi}\frac{\omega v}{kT}\right)$$

and determine an expression for the vibrational partition function. [4 Marks]

Assuming that the rotational energies for this heteronuclear, diatomic rigid-rotator molecule are $E(J) = hcBJ(J+1)$, $(J = 0, 1, 2, \ldots)$, show that the population is then approximated by:

$$N_{v,J} = \frac{N(2J+1)}{Q(T)_{vib} Q(T)_{rot}} \exp\left(-\frac{h}{kT}\left(\left(\frac{\omega v}{2\pi}\right) + cBJ(J+1)\right)\right)$$ [4 Marks]

and that the rotational partition function can be approximated by

$$Q(T)_{rot} \cong \frac{kT}{hcB}$$ [4 Marks]

Thus determine an expression for the vibration/rotation level population. [4 Marks]

Find the value of J for which this population maximises and sketch the expected spectrum that you would observe at temperatures typical of planetary atmospheres. Define the rotational temperature of a gas. [4 Marks]

4. The intensity emitted vertically by a single isothermal atmospheric layer at frequency $\bar{\nu}$ is given by:

$$I(\bar{\nu}) = B[\bar{\nu}, T_A]\{1 - \exp(-\tau(\bar{\nu}))\},$$

where T_A is the atmospheric temperature and $\tau(\bar{\nu})$ is its opacity. Assuming that the Rayleigh-Jeans approximation can be used, show that the measured intensity can be written as an effective brightness temperature $T_m(\bar{\nu})$, and hence re-formulate the above equation in temperature units. [3 Marks]

A planet has a surface temperature of 220 K and an atmospheric temperature which goes from 220 K at the surface through a temperature minimum at 180 K to a maximum of 280 K at the top. It is in hydrostatic equilibrium so that,

$$\frac{dP}{dz}=-gmN$$

where P, N, m, and g are, respectively, the pressure, molecular number density, mean molecular weight, and acceleration due to gravity at height, z. Assuming the perfect gas law, $P=NkT$, where k is the Boltzmann constant and T the temperature, show that the change in molecular number density with altitude is given by

$$\frac{dN}{dz}=-N\left(\frac{mg}{kT}+\frac{1}{T}\frac{dT}{dz}\right).$$ [5 Marks]

Define a positive lapse rate as used in planetary atmospheres. [2 Marks]

Show that, in a non-isothermal atmosphere with a constant value of -dT/dz = Γ, the molecular number density becomes:

$$N=N_S\left(\frac{T}{T_S}\right)^{-\left(1-\frac{mg}{k\Gamma}\right)}$$, where N_S and T_S are the surface values. [4 Marks]

If the planet's atmosphere contains a well mixed absorber with a single isolated line, sketch the emission spectrum (in temperature units) that you would expect to observe as a function of absorber strength for;

a. A downward looking satellite
b. An upward looking observer on the planet's surface

Your sketch should indicate the relative linewidths that you would observe. [6 Marks]

5. Discuss **briefly** the different uses of Nadir and Limb sounding geometries. [4 Marks]

It can be shown that the intensity emitted vertically by a stratified atmosphere is given by

$$I(\bar{\nu})=\int B(\bar{\nu},T(z))\kappa(z,\bar{\nu})\exp\left(-\int_0^z \kappa(z',\bar{\nu})dz'\right)dz,$$

where $B(\bar{\nu}, T(z))$ is the Planck function at temperature $T(z)$ and $\kappa(z, \bar{\nu})$ is the absorption coefficient at frequency $\bar{\nu}$; all defined at altitude z. $\alpha(z,\bar{\nu}) = \exp\left(-\int_0^z \kappa(z',\bar{\nu})dz'\right)$ is the atmospheric transmittance; show that the expression for the intensity can be reduced to

$$I(\bar{\nu}) = \int B(\bar{\nu}, T(z)) W(z, \bar{\nu}) dz$$

and determine an expression for $W(z, \bar{\nu})$. [6 Marks]

For a single Doppler broadened spectral line of strength S centered at frequency $\bar{\nu}_o$, the absorption coefficient $\kappa(\bar{\nu})$ is,

$$\kappa(\bar{\nu}) = S \frac{2(\ln 2)^{1/2}}{\pi w_D} \exp\left(-\frac{4 \ln 2 (\bar{\nu} - \bar{\nu}_o)^2}{w_D^2}\right)$$

where w_D is the Doppler line width. For a uniformly mixed absorber in hydrostatic equilibrium, $dp/dz = -g\rho$, g is acceleration due to gravity and ρ is the density. Show that

$$\alpha(\bar{\nu}) = \exp(-\beta p)$$

and, determine an expression for β. [4 Marks]

With a change of variable from z to $y = -\ln(p)$, the intensity can be written as:

$$I(\bar{\nu}) = \int B(\bar{\nu}, T(y)) \frac{d\alpha(y, \bar{\nu})}{dy} dy = \int B(\bar{\nu}, T(y)) W(y, \bar{\nu}) dy$$

Determine the form of $W(y)$ and sketch it as a function of p/p_o where p_o is the pressure where $W(y)$ maximizes.

The equivalent expression for a pressure broadened line is:

$$W(y) = 2\left(\frac{p}{p_o}\right)^2 \left\{\exp - \left(\frac{p}{p_o}\right)^2\right\}$$

Overlay this function on your plot and discuss the implications of these results. [6 Marks]

6. Discuss two modeling approaches leading to the extraction of atmospheric parameters from spectral measurements. [4 Marks]

Outline the problems associated with extracting atmospheric parameters from the measured spectral emission. [6 Marks]

Outline two inversion methods that are used to give approximate results. [10 Marks]