Fundamentals of atmospheric chemistry and astrochemistry

Problems for Lectures 1-3: Astrochemistry

Q1. (a) Use the Rydberg equation to calculate the first transition energy in the Lyman, Balmer, Paschen, and Brackett series of atomic hydrogen, which terminate on $n = 1$, 2, 3, and 4, respectively.

(b) Which of these series can be observed in atmospheric windows?

Q2. The Hα transition is the transition from the n=3 to n=2 level in atomic hydrogen. The transition has been used to determine the rotation speed of Jupiter.

(a) Use the Rydberg equation to calculate the wavelength of the Hα transition to 3 decimal places.

(b) The rotation speed of a point on the surface of Jupiter at the equator is 43 000 km h^{-1}. Calculate the Doppler shifts for the Hα line observed from points on the extreme left and extreme right of Jupiter's equator, as viewed from earth. What would be the Doppler shift for a point observed in the centre of the planet as viewed from earth.

Q3. The microwave spectrum of an interstellar gas cloud has been recorded in the region containing CO transitions. The observed intensity ratio R(1)/R(0) for the first two lines from the R branch of the CO rotational spectrum is 1.10. Calculate the temperature of the cloud.

Q4. The star Rigel has a surface temperature of 11 000 K. Calculate the relative populations of the two levels involved in the Hα transition at this temperature.

Q5. (a) Briefly discuss the events leading to star formation within a molecular cloud.

(b) During protostar formation within a molecular gas cloud, molecular dissociation occurs as the temperature rises, followed by atomic ionization at even higher temperatures. Calculate the temperatures at which the following bonds would dissociate. Bond dissociation energies are given in parentheses.

(i) N-N (943 kJ mol^{-1})
(ii) C=O (1075 kJ mol^{-1})
(iii) C=C (612 kJ mol^{-1})
(iv) C-C (348 kJ mol^{-1})

(v) C-H (415 kJ mol^{-1})

(c) Calculate the temperatures at which the following atoms would be ionized. Ionization potentials are given in parentheses.

(i) H (13.6 eV)
(ii) He (24.59 eV)
(iii) C (11.26 eV)
(iv) He+ (54.51 eV)

Q6. The mass of the sun is 2 x 10^{30} kg. Calculate the smallest diameter of a (spherical) interstellar gas cloud with a density of 1000 cm^{-3} that could collapse to form a star with one solar mass.

Q7. Calculate the collision frequency for hydrogen molecules (collision cross section 0.27 nm^2) in

(a) A sample of H_2 gas at atmospheric pressure.

(b) A giant molecular cloud with $n = 10^5$ cm^{-3} and T = 40 K.

(c) The diffuse interstellar medium, with $n = 10$ cm^{-3} and $T = 10$ K.

[Note that for collisions between particles of the same type, a factor of ½ is required in the expression for the collision frequency to avoid double counting of collisions.]

Q8. A simple model reaction scheme for the hydrogen chemistry occurring within an interstellar gas cloud is given below.

$$H + H \xrightarrow{\text{dust grain}} H_2 \qquad k_1$$
$$H_2 \xrightarrow{h\nu \text{ or cr}} H_2^+ + e^- \qquad k_2$$
$$H_2^+ + H_2 \longrightarrow H_3^+ + H \qquad k_3$$
$$H_3^+ + CO \longrightarrow HCO^+ + H_2 \qquad k_4$$

(a) Explain the chemistry occurring in each step in the reaction sequence.

(b) Apply the steady state approximation to $[H_2^+]$ and $[H_3^+]$ to obtain an expression for the overall rate of formation of HCO^+.

(c) The steady-state concentration of H_3^+ is 2 x 10^4 cm^{-3}. The astronomical observation for the column density (the density of H_3^+ along the line of sight) is 3 x 10^{24} cm^{-2}. Calculate the diameter of the molecular cloud in (i) metres, and (ii) light years.

Q9. A simple model reaction scheme for some of the reactions involving the CH^+ ion within a molecular gas cloud is shown below.

$$C^+ + H_2 \rightarrow CH^+ + H \qquad k_1$$
$$CH^+ + N \rightarrow CN^+ + H \qquad k_2$$
$$CH_2^+ + H \rightarrow CH^+ + H_2 \qquad k_3$$
$$C + CH^+ \rightarrow C_2^+ + H \qquad k_4$$

(a) Use the steady-state approximation to derive an expression for the concentration of CH^+.

(b) Define the impact parameter for an ion-molecule collision.

(c) At a given impact parameter, for which pair of reactants in the four elementary reactions above will the orbital angular momentum ***L*** be the highest? Calculate the constant of proportionality between ***L*** and b for each of reactions 1 – 4 at a temperature of 50 K.

(d) Which reaction is likely to be the rate determining step? Explain your answer.

Q10. Assuming the locked dipole approximation, the long-range part of the effective potential for an ion-molecule reaction is given by

$$V_{\text{eff}} = -\frac{\alpha q^2}{8\pi\varepsilon_0 r^4} - \frac{\mu_D q}{4\pi\varepsilon_0 r^2} + \frac{\mu v_{\text{rel}}^2 b^2}{2r^2}$$

(a) Explain the origin of the three terms in this expression.

(b) Sketch the form of the potential.

(c) Determine the radial position r_0 at which the potential is a maximum.

(d) For a given collision energy, E_{coll}, explain how V_{eff} could be used to determine a maximum impact parameter b_{max} for the reaction, and therefore a reaction cross section $\sigma_c(E)$. You *do not* need to calculate b_{max} or $\sigma_c(E)$.

(e) Explain (with equations where appropriate) how $\sigma_r(E)$ could be used to obtain the thermal rate constant for the reaction.