

Chemistry 412

Physical Chemistry

Problem Set 2 - 25 Points

Due: Wednesday, Sept. 14. Read Chapters 2 and 3 in “Quantum Chemistry & Spectroscopy” by Engel. Also, please read or review section 1-4, section 1-5, chapter 4 and chapter 5 in “Applied Mathematics for Physical Chemistry” by Barrante. Complete the following problems. Please SHOW ALL OF YOUR WORK on mathematical problems.

1. (2 pts) *Barrante*, Chapter 1, Problem 4
2. (2 pts) *Barrante*, Chapter 5, Problem 1, (a)-(e) only.
3. (2 pts) *Barrante*, Chapter 5, Problem 2, (h), (j), (m), (r) only (be sure to indicate the number of the integral used and substitutions)
4. (2 pts) *Barrante*, Chapter 5, Problems 3(f)-(i).
5. (2 points) *Engel*, Chapter 2, Problem P2.12 Which of the following are eigenfunctions of the operator $\frac{d^2}{dx^2}$? If they are eigenfunctions, what is the eigenvalue?

- (a) $ae^{-3x} + be^{3ix}$ (c) e^{-ix} (e) e^{-ix^2}
(b) $\sin^2 x$ (d) $\cos ax$

6. (3 points) *Engel*, Chapter 2, Problem P2.27 Find the result of operating with: $(\frac{1}{r^2})(\frac{d}{dr})(r^2\frac{d}{dr} + \frac{2}{r})$ on the function Ae^{-br} . What must the values of A and b be to make this function an eigenfunction of the operator?
7. (3 points) *Engel*, Chapter 2, Problem P2.28 Normalize the set of functions $\phi_n(\theta) = e^{in\theta}$, $0 \leq \theta \leq 2\pi$, n is an integer.
8. (3 pts) *Engel*, Chapter 1, Problem P1.7 Show that the energy density radiated by a blackbody

$$\frac{E_{total}(T)}{V} = \int_0^\infty \rho(\nu, T) d\nu = \int_0^\infty \frac{8\pi h\nu^3}{c^3(e^{h\nu/kT} - 1)} d\nu$$

depends on the temperature as T^4 . Using your result, calculate the energy density radiated by a blackbody at 1350. K and 5250. K. (NOTE: see pg 15 in text for a description of how to do this - more details in the book).

9. (3 pts) In the previous homework, you calculated the average power per unit area reaching the surface of the planet Mercury to be about 2230 W/m². Some of this is reflected back into space, the rest is absorbed by the surface (Mercury has no atmosphere). The fraction of incoming radiation reflected back into space is reported as the planet's albedo. Mercury has an albedo of 0.068.

Calculate the expected surface temperature of Mercury, T_{ground} . We can do this by recognizing two things (1) the surface of the planet radiates heat back out into space like a black body and (2) the energy flux (power) of the incoming radiation is equal to the total energy flux of the radiation going back into space.

$$P = \sigma T_{ground}^4 \qquad \sigma = 5.67 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$$

Compare your result to the reported mean surface temperature (cite).

10. (3 points) *Engel*, Chapter 2, Problem P2.15 Show by carrying out the integration that $\sin(m\pi x/a)$ and $\cos(m\pi x/a)$, where m is an integer, are orthogonal over the interval $0 \leq x \leq a$. Would you get the same result for the interval $0 \leq x \leq 3a/4$? Explain your result.