Student Name_____

Chemistry 881 October 3, 2001

Examination 2

1. (10 points) Solve the equation

$$\frac{d^2x}{dt^2} + \omega^2 x(t) = 0$$

Subject to the initial conditions $x(0) = A$ and $\frac{dx}{dt} = 0$ at $t = 0$

2. (20 points) In each case, show that $f(x)$ is an eigenfunction of the operator given. Find the eigenvalue.

| | $\hat{A}$ | $f(x)$ |
|---|---|---|
| (a) | $\frac{d^2}{dx^2}$ | $\cos \omega x$ |
| (b) | $\frac{d}{dt}$ | $e^{i\omega t}$ |
| (c) | $\frac{d^2}{dx^2} + 2\frac{d}{dx} + 3$ | $e^{\alpha x}$ |
| (d) | $\frac{\partial}{\partial y}$ | $x^2 e^{6y}$ |

3. (20 points) Use the free electron model for the pi electrons in hexatriene and show that the first electronic transition is predicted to occur at $2.8 \times 10^{4} cm^{-1}$. The length of hexatriene can be estimated to be 867 pm.

4. (15 points) The force constant of $^{79}Br^{79}Br$ is 240 Nm-1. Calculate the fundamental vibrational frequency and the zero point energy of $^{79}Br^{79}Br$ in $cm^{-1}$ .

5. (5 points)Show that the moment of inertia for a rigid rotator can be written as $I = \mu R^2$ where $R = R_1 + R_2$ (the fixed separation between the two masses) and $\mu$ is the reduced mass.

6. (15 points) In the infrared spectrum of $H^{79}Br$, there is a series of lines separated by $16.72cm^{-1}$. Calculate the values of the moment of inertia and the internuclear separtion in $H^{79}Br$.

7. (15 points) Evaluate the integral

$$I = \int_0^{\pi} \cos^2\theta \sin^3\theta d\theta$$

by letting $x = \cos\theta$