CHEM 571A - Problem Set #3

Due Friday September 13th

1. *McQuarrie 4-11:* Evalutate the commutator $[\hat{A}, \hat{B}]$, where $\hat{A}$ and $\hat{B}$ are given below

	$\hat{A}$	$\hat{B}$
(a)	$\frac{d^2}{dx^2}$	x
(b)	$\frac{d}{dx} - x$	$\frac{d}{dx} + x$
(c)	$\int_0^x dx$	$\frac{d}{dx}$
(d)	$\frac{d^2}{dx^2} - x$	$\frac{d^2}{dx^2} + x^2$

2. *McQuarrie 5-14:* The force constant of $^{35}C^{35}Cl$ is 319 $N \cdot m^{-1}$. Calculate the fundamental vibrational frequency and the zero-point energy of $^{35}C^{35}Cl$ (in the harmonic approximation).

3. *McQuarrie 5-19:* The vibrational term of a diatomic molecule is given to good approximation by

$$G(\nu) = \left(\nu + \frac{1}{2}\right)\tilde{\omega}_e - \left(\nu + \frac{1}{2}\right)^2 \tilde{x}_e\tilde{\omega}_e$$

where ν is the vibrational quantum number. Show that the spacing between adjacent levels ΔG is given by

$$\Delta G = \tilde{\omega}_e\{1 - 2\tilde{x}_e(\nu + 1)\}$$

Also show that the maximum vibrational quantum number is given by

$$\nu_{max} = \frac{1}{2\tilde{x}_e} - 1$$

Use the above result to compute the dissociation energy, D_e, of the molecule.'

4. *McQuarrie 5-22:* Show that $\psi_0(x)$ and $\psi_1(x)$ for the harmonic oscillator are orthogonal.