Chem 442: Homework for lecture L32

(only turn in **BOLD** assignment first lecture next week of classes; do <u>all</u> assignments)

1. **Turn in** Write down the Born – Oppenheimer wavefunction $\psi_{tot}(\vec{r}, \vec{R}_A, \vec{R}_B)$ for H_2^+ when the molecule is in the "ground electronic, ground vibrational, and 1st excited rotational state." Use the MO basis for the electronic part. $\vec{r}$ is the coordinate of the electron, and $\vec{R}_n$ with n=A or B are the two coordinates of the H^+ nuclei. So for example, the distance from the electron to nucleus A is $r_{1A} = |\vec{r} - \vec{R}_A|$, and the distance between the two nuclei is $R=|\vec{R}_B - \vec{R}_A|$, etc.
   Use actual written-out functions for $\psi_0(r_{1A}, r_{1B}, spin)$, $\chi_m(R)$ and $Y_{JM_J}(\theta, \varphi)$. Except for the spin parts α and β, your function should be spelled out in terms of simple known function like Gaussians, exponentials, cosines, etc. Neglect normalization. Don't forget about the spin wavefunction You can leave the constants undefined, like k in $1s_A(r_{1A}) \sim e^{-kr_{1A}}$ and ω in $e^{-m\omega R^2/2\hbar}$.