

Quantum Mechanics and Spectroscopy  
CHEM 3PA3  
Assignment 21

Name: \_\_\_\_\_

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1. Because the chemical bond in CO (carbon monoxide) is so strong, it is sometimes interesting to measure rotational spectra for several different isotopes. For example, we could measure the rotational spectrum for  $^{12}\text{C}-^{16}\text{O}$  and  $^{14}\text{C}-^{18}\text{O}$ . What is the difference between the rotational energy levels of these isotopes?
2. The harmonic oscillator is an excellent approximation to the vibrations in CO. The lowest-energy electric-dipole-allowed vibrational excitation of the CO molecule is associated with absorbing photons with frequency  $6.42 \times 10^{13}$  Hz. The equilibrium bond length of CO is  $1.28 \times 10^{-10}$  m. What would be the energy of the ground state if one tries to obtain an approximate ground state energy with the variational principle using the following trial wavefunction?

$$\psi(r) = Ae^{-\alpha(r-1.128 \times 10^{-10}\text{m})^2}$$

3. Assume  $r_e = 113.1$  pm,  $k = 1902$  N/m for all isotopes of CO. What is  $\Delta H^0$  (in Joules) of the reaction  $^{13}\text{C}^{17}\text{O} + ^{12}\text{C}^{16}\text{O} \longrightarrow ^{12}\text{C}^{17}\text{O} + ^{13}\text{C}^{16}\text{O}$ ? Assume that all molecules are harmonic oscillators in their vibrational ground states. You only need to consider the differences in vibrational energy between the different isotopes.
4. Label each molecule as: **S** spherical top, **P** prolate symmetric top, **O** oblate symmetric top, or **A** asymmetric top.  

(a) Propyne	(c) Carbon tetrachloride
(b) 1-butyne	(d) Coronene
5. Draw the molecular orbital diagram for  $\text{BH}_3$ .
6. You are given an excited state of the Lithium atom, with electron configuration  $1s^1 2s^1 2p^1$ , and told that  $L = 1$ ,  $S = 3/2$ , and  $J = M_J = 5/2$ . Write a Slater determinant wavefunction for this state. Write the Slater determinant in the long form (as a matrix), showing the dependence on the spatial and spin coordinates of all 3 electrons.