



Lesson: MOLECULAR SPECTROSCOPY

PROBLEM SHEET: QUESTIONS

1. (◆◆◆) The following transitions are detected in the microwave spectrum of the vibrational ground state of the CO molecule

$J \rightarrow J'$	$0 \rightarrow 1$	$1 \rightarrow 2$	$2 \rightarrow 3$	$3 \rightarrow 4$	$4 \rightarrow 5$
ν (MHz)	115271.20	230537.97	345795.90	461040.70	576267.80

It is also observed the $J = 0 \rightarrow 1$ transition of the $v = 1$ vibrational state at 114221.2 MHz. Calculate B_e , r_e y $D_{e,r}$.

2. (◆◆◆) Calculate the ω_e and $\omega_e \chi_e$ constants of the HCl molecule using the following IR transitions

$v \rightarrow v'$	$0 \rightarrow 1$	$0 \rightarrow 2$	$0 \rightarrow 3$	$0 \rightarrow 4$	$0 \rightarrow 5$
$\tilde{\nu}$ (cm ⁻¹)	2885.9	5668.0	8347.0	10923.1	13396.5

3. (◆◆◆) The fundamental band origin of the CO molecule is observed at 2143 cm⁻¹ and the first overtone at 4260 cm⁻¹. Calculate the ω_e and $\omega_e \chi_e$ constants, D_e and D_0 .
4. (◆◆◆) Deduce expressions of the wavenumbers of the R and P branches spectral lines for a diatomic molecule.

Difficulty level: (◆◆◆) Easy, (◆◆◆) Normal, (◆◆◆) To think a bit.

PROBLEM SHEET: SOLUTIONS

Question 1 $\Rightarrow B_e = 57898 \text{ MHz}$, $r_e = 1.128 \text{ \AA}$, $D_{e,r} = 0.18 \text{ MHz}$

Question 2 $\Rightarrow \omega_e = 2988.7 \text{ cm}^{-1}$, $\omega_e \chi_e = 51.6 \text{ cm}^{-1}$

Question 3 $\Rightarrow \omega_e = 2169 \text{ cm}^{-1}$, $\omega_e \chi_e = 13 \text{ cm}^{-1}$, $D_e = 11.22 \text{ eV}$, $D_0 = 11.1 \text{ eV}$
