Chemistry II: Introduction to Molecular Spectroscopy

Video Tutorials 2: Vibrational (Infrared) spectroscopy

Problem 1: The following molecules have pure rotational spectrum, infrared spectrum or both. Identify them accordingly.

CO		CH_2Cl_2	
CO_2		NH_3	
C_2H_6		CH_3CHO	
CH_4		Benzene	
Trans-dichloro ethylene		Ozone	
Acetylene		H_2O_2	
propyne			

Problem 2:

Determine the moment of inertia of water molecule about its symmetry axis (passing through oxygen and bisecting the HOH bonds OH bond distance is 95.7 picometers and the HOH bond angle is 104.5 degrees

Problem 3:

The fundamental vibrational frequency of hydrogen molecule is 4401.2 cm^{-1}. What are the vibrational frequencies of HD and D_2 if the force constant of all the three molecules are approximately the same?

Problem 4.

The Morse potential is given by the expression

$$V(r) = D\left[1 - e^{-\alpha(r-r_e)}\right]^2.$$

Show that in the limit of small displacements this is the same as harmonic approximation. Identify the harmonic frequency. Also show that the asymptotic value is D. what are the interpretations for the parameters in the Morse potential?

Problem 5

Determine the fraction of molecules of in the v=1, 2 and 3 states relative to the ground state v=0 for the molecule bromine monofluoride is 669.7 cm^{-1}. T=1000 K.

Problem 6:

The vibrational frequency ω_e and the anharmonicity constant $\omega_e x_e$ for BrF have been found from experiments to be about 669.7 and 3.869 cm-1, respectively. Calculate the first four Morse oscillator energy levels for this molecule and transition frequencies for the transitions $\mathrm{v} = 0 \rightarrow 2$ and $\mathrm{v} = 1 \rightarrow 3$

Problem 7 (advanced)

Obtain all the simple harmonic oscillator wave functions for n=0 to n=3. Determine why the selection rule for vibrational spectrum of a harmonic oscillator contains only one line with the selection rule $\Delta v = \pm 1$

Problem 8

For the molecule Boron trifluoride, calculate the three principal moments of inertia and identify the type. Calculate all energy levels of this molecule for J up to and including 3.

Problem 9

The rotational spacing between successive lines of HCl is 20.8 cm^{-1}.

a) Calculate the bond distance

b) Determine the number of molecules in the level J = 4 relative to J = 3.

c) Determine the level in which there is maximum population. T=300 K may be assumed.

Problem 10

Classify each of the molecules as spherical, symmetric, asymmetric tops.

CBr_4, $CHCl_3$, SF_6, CH_2Cl_2, O_3, HCN, C_2H_4

- Enjoy your learning and send me problems that you may want to solve in elementary spectroscopy. Please remember learning is reinforced through problem solving and not the other way around—i.e., by solving problems you don't necessarily learn new concepts. You have to read, think about it and discuss that. Online learning through this course is by self-motivation only. All the best. Mangala Sunder