

2011/2012 FIRST SEMESTER LECTURE GUIDE ON SELECTED TOPICS

CHM 333 – ATOMIC AND MOLECULAR SPECTROSCOPY

PART A

Topic(s): Rotational and vibrational spectra of diatomic molecules - application to IR and Raman spectroscopy

1. Outline the differences between atomic and molecular spectroscopy
2. General features of
3. a) Vibrational spectroscopy

The classical harmonic oscillator – force constant (explanation on bond strength, stretching and compression of bonds)

Group frequencies, state populations for selected diatomic molecules,

Fundamental and overtones transitions, Morse potential

IR absorption spectroscopy – instrumentation, molar absorption coefficient, calculations involving vibrational frequencies

b) Rotational spectroscopy

Rotational energy and angular momentum quantum number j , moment of inertia.

Rotational vibrational spectral of selected diatomic showing the R branch and P branch

FTIR

Raman spectroscopy

4. Characteristics of spectra lines and intensities
5. Selection rules

