

# CHM 3411 Problem Solving Session, 4-18-2018

Chapter 12: Rotational and Vibrational Spectra

# To know for exam 3

- Selection rules, gross and specific, for:
  - Microwave spec. (spherical tops, symmetric tops, linear molecules), rotational Raman, IR specs, Vibrational Raman
- Equation for  $\tilde{B}$  ( $\tilde{B} = \frac{\hbar}{4\pi cI}$ ) and for  $\tilde{\nu}$  ( $\tilde{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{\mu}}$ )
- Equation for  $E(v,J)$ :  $E(v, J) = hc\tilde{B}J(J + 1) + \left(v + \frac{1}{2}\right) hc\tilde{\nu}$
- Definition of rotational, vibrational, and vibrational-rotational terms ( $\tilde{F}, \tilde{G}, \tilde{S}$ )
- Equation for moment of inertia of diatomic ( $I = \mu R^2$ ; also know equation for  $\mu$ )
- 3 types of radiative processes (stimulated absorption, etc.)
- Definition of transition dipole moment and transition dipole operator

# Be able to explain

Absorption vs scattering of radiation

Stark effect

Relationship between nuclear statistics and rotational states

Anharmonicity

Centrifugal distortion

$D_e$  vs  $D_o$

P, Q, and R branches; O and S branches

Stokes vs Antistokes

# Be able to

- Determine  $I$  and the moment of inertia from a microwave, rotational Raman, IR, or vibrational Raman spectrum
- Determine  $\tilde{\nu}$  and the force constant,  $k$ , from the vibrational or vibrational Raman spectrum
- Determine  $D_0$  from an IR spectrum
- Determine  $R_e$  from a microwave or IR spectrum of a diatomic
- Determine geometric parameters for a larger molecule with sufficient symmetry using a table of molecular symmetries and different isotopomers
- Calculate temperature from a microwave or IR spectrum

- Which have a pure microwave spectrum?
  - $\text{H}_2$ ,  $\text{HCl}$ ,  $\text{CH}_4$ ,  $\text{CH}_3\text{Cl}$ ,  $\text{CH}_2\text{Cl}_2$
- Which have a rotational Raman spectrum?
  - $\text{H}_2$ ,  $\text{HCl}$ ,  $\text{CH}_4$ ,  $\text{CH}_3\text{Cl}$
- Which may show an IR spectrum? Can you predict which vibrational modes are IR active?
  - $\text{H}_2$ ,  $\text{HCl}$ ,  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ?

# Selected Exercises to work on

- 12C.1(b)
  - 12C.7(b)
  - 12D.2(b)
  - 12D.5(a)
  - 12D.6(b)
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- Problems: 12D.4, 12D.8