

## Molecular Vibrations

### Read:

- Cotton, *Chemical Applications...*, Chapter 10.
- Harris & Bertolucci, *Symmetry and Spectroscopy...*, Chapter 3, pp. 93-117; 135-167; 170-201.

## Diatomic Molecules

The harmonic oscillator Hamiltonian is

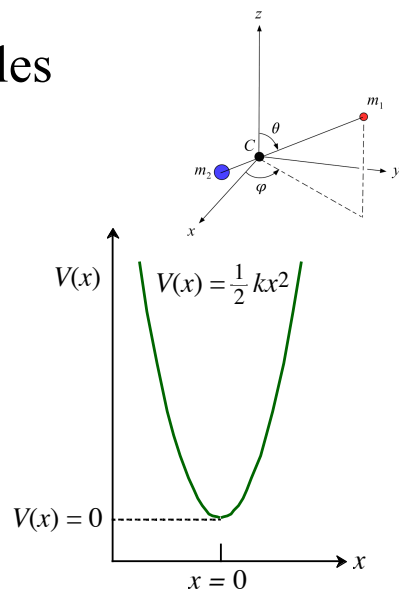
$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \varphi = E\varphi \quad V(x) = \frac{1}{2} kx^2$$

$x$  = distance from  $x_0$

$$\left( \text{Hooke's Law: Force} = F = -\frac{dV(x)}{dx} = -kx \right)$$

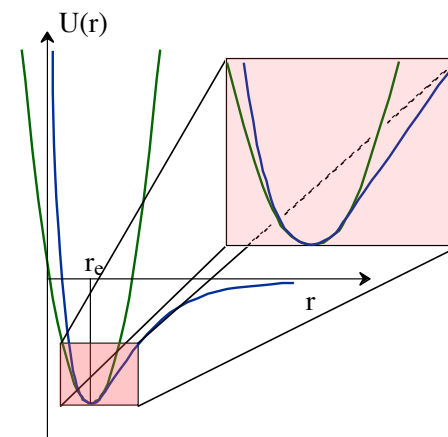
## Diatomic Molecules

- The effective potential,  $V(x)$ , in which the nuclei move is determined by the electronic energy & nuclear-nuclear repulsion.
- $k$ , the force constant, is linked to vibrational frequency,  $\nu = (1/2\pi)(k/\mu)^{1/2}$



## Real vs. Harmonic Potential

Harmonic (quadratic) potential is an approximation of the true ground state binding curve for the diatomic molecule.



## Normal Coordinate for diatomics

The Hamiltonian is rewritten (change of variables to mass weighted coordinate):

$$-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \Rightarrow -\hbar^2 \frac{d^2}{dq^2} + \frac{1}{2} \lambda q^2$$

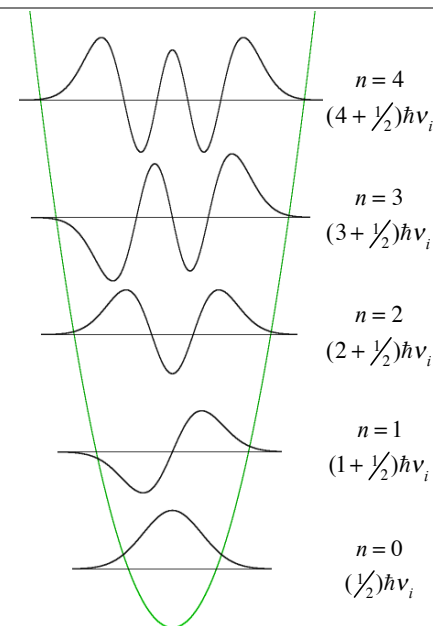
$$\mu = \frac{m_1 m_2}{m_1 + m_2} \quad q = \sqrt{\mu} x; \quad \lambda = k/\mu; \quad V(q) = \frac{1}{2} \lambda q^2$$

$$\text{frequency } \nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} = \frac{1}{2\pi} \sqrt{\lambda}$$

## Harmonic Oscillator Wavefunctions

$$\psi_i(n) = N_i e^{-(\alpha_i/2)Q_i^2} H_n(\sqrt{\alpha_i} Q_i)$$

$$\alpha_i = 2\pi n_i \mu / \hbar$$



## Normal Coordinates

- Expressed in terms of normal coordinates, the vibrational potential energy function is diagonal (contains no cross terms):

$$U = U_{eq} + \frac{1}{2} \sum_{k=1}^{3N-6} \lambda_k Q_k^2$$

There are no terms involving  $Q_i Q_j$

## Normal Coordinates for Polyatomics

- For polyatomics, there exists a set of normal coordinates in which the vibrational Hamiltonian is separable

$$\mathcal{H}_{vib} = \sum_{k=1}^{3N-6} \mathcal{H}_k; \quad \mathcal{H}_k = -\frac{\hbar^2}{2} \frac{\partial^2}{\partial Q_k^2} + \frac{1}{2} \lambda_k Q_k^2$$

$Q_k$  are mass-weighted coordinates

- Energies are summed:

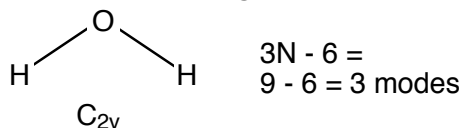
$$\text{each mode: } E_i = (n_i + \frac{1}{2})h\nu_i \quad \text{Total: } E_{tot}^{vib} = \sum_{i=1}^{3N-6} E_i$$

- Wavefunctions are products of wavefunctions of modes:

$$\psi_1(n_1)\psi_2(n_2)\cdots\psi_{3N-6}(n_{3N-6}) = \prod_{i=1}^{3N-6} \psi_i(n_i)$$

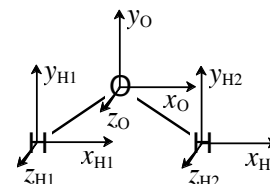
## Normal Modes

The “normal modes” of vibration are those which correspond to motions along “normal coordinates”. Such normal coordinates transform as irreducible representations of the applicable point group, but are generally combinations of symmetry adapted internal coordinates. For example, consider H<sub>2</sub>O. To what I.R.s do the normal modes belong?



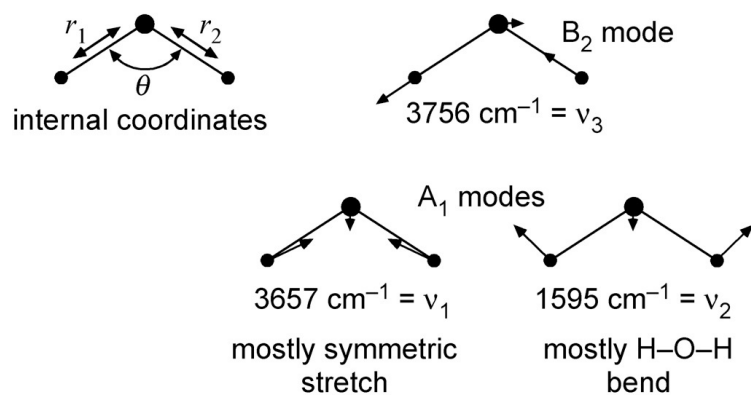
## Determining Normal Mode Symmetries

- Find reducible rep. for all nuclear motions



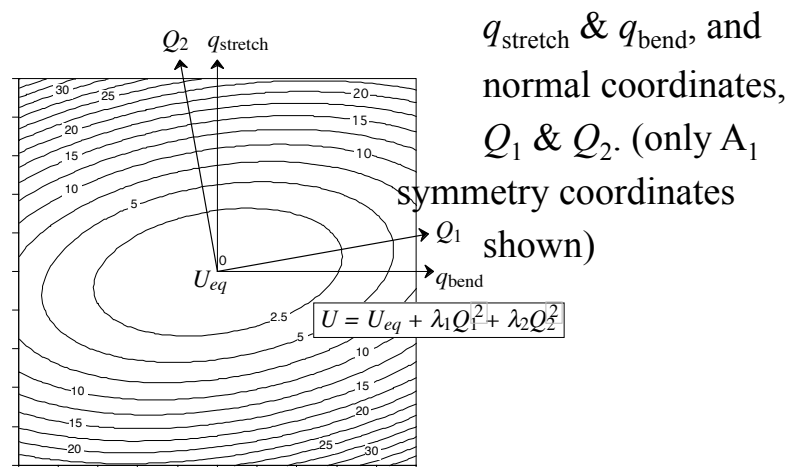
- Eliminate translations and rotations (6 for nonlinear molecules, 5 for linear molecules). This guarantees that normal modes involve no net translation or rotation of center of mass.

## Normal Coordinates and Symmetry Coordinates

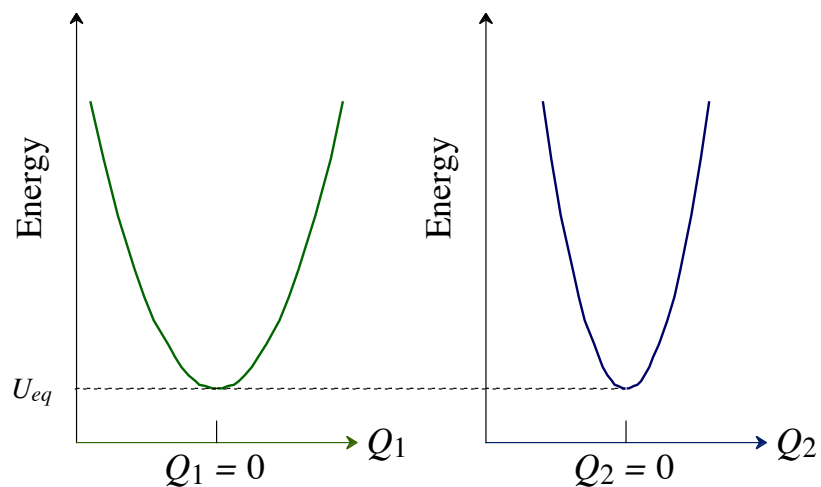


Frequencies are for H<sub>2</sub><sup>16</sup>O.  
For D<sub>2</sub><sup>16</sup>O, ( $\nu_1, \nu_2, \nu_3$ ) = (2669, 1178, 2788 cm<sup>-1</sup>)

For the two A<sub>1</sub> modes of H<sub>2</sub>O, the potential energy surface in terms of internal coordinates,



## 1-D Slices Through 2-D Potential Surface



## Harmonic Oscillator Wavefunctions

- For each mode,  $i$ ,  $\psi_i$  has the form

$$\psi_i(n) = N_i e^{-(\alpha_i/2)Q_i^2} H_n(\sqrt{\alpha_i}Q_i); \quad \alpha_i = 2\pi n_i \mu / \hbar$$

$$H_0(x) = 1; \quad H_1(x) = 2x; \quad H_2(x) = 4x^2 - 2;$$

$$H_3(x) = 8x^3 - 12x; \quad H_4(x) = 16x^4 - 48x^2 + 12$$

For even(odd)  $n$ ,  $H_n(x)$  is an even(odd) function.

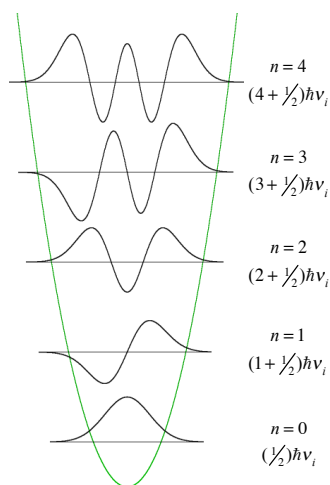
$$H_n(\sqrt{\alpha_i}Q_i) \xrightarrow{\hat{R}} +H_n(\sqrt{\alpha_i}Q_i) \text{ for even } n.$$

$$\text{and } H_n(\sqrt{\alpha_i}Q_i) \text{ transforms like } Q_i \text{ for odd } n.$$

## Fundamentals, Overtones, Combinations

A molecule may be excited with multiple vibrational quanta. e.g., for H<sub>2</sub>O three numbers specify the number of quanta in each mode.

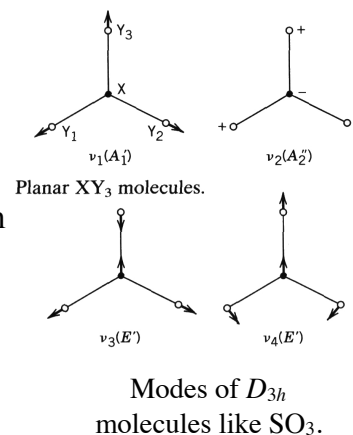
- Fundamentals: 100 010 001  
A<sub>1</sub> A<sub>1</sub> B<sub>2</sub>
- Overtones: 200 020 002  
A<sub>1</sub> A<sub>1</sub> A<sub>1</sub>
- Combinations: 110 101 011  
A<sub>1</sub> B<sub>2</sub> B<sub>2</sub>



## Degenerate Modes

A molecule with sufficiently high symmetry will have some vibrational modes that are degenerate.

- When all modes are in their ground states, their contribution to the total vibrational wavefunction's symmetry is still totally symmetric.
- Overtones (in which there are two or more quanta of vibrational excitation) must be handled with care.



If two modes,  $i$  &  $j$ , form a basis for a degenerate representation, then  $\lambda_i$  and  $\lambda_j$  are equal (i.e., the modes have the same frequency). Then,

$$\hat{R}Q_i = aQ_i + bQ_j ; \hat{R}Q_j = cQ_i + dQ_j$$

$$\Gamma(R) = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \text{ is an orthogonal matrix}$$

$$\therefore a^2 + b^2 = c^2 + d^2 = a^2 + c^2 = c^2 + d^2 = 1; \\ ac + bd = ab + cd = 0.$$

$$\lambda_i (\hat{R}Q_i)^2 + \lambda_i (\hat{R}Q_j)^2 = \lambda_i \left[ \begin{array}{l} a^2 Q_i^2 + b^2 Q_j^2 + 2ab Q_i Q_j \\ + c^2 Q_i^2 + d^2 Q_j^2 + 2cd Q_i Q_j \end{array} \right] \\ = \lambda_i (Q_i^2 + Q_j^2) \quad \leftarrow 2(ab + cd)Q_i Q_j = 0$$

## The Result:

The total potential,  $U$ , is not changed under the action of a symmetry operation. Total wavefunction is unchanged too:

when  $\alpha_i = \alpha_j$ ,

$$e^{-\frac{\alpha_i}{2} Q_i^2} e^{-\frac{\alpha_j}{2} Q_j^2} = e^{-\frac{\alpha_i}{2} (Q_i^2 + Q_j^2)} \xrightarrow{\hat{R}} e^{-\frac{\alpha_i}{2} (Q_i^2 + Q_j^2)}$$

$\psi_{\text{vib.}}$  is therefore unchanged in the ground state

(At the bottom p. 325 in Cotton, this is not at all clear.)

- **Conclusion:** All molecules' vibrational wavefunctions belong to the totally symmetric representation for the appropriate point group when the molecule is in its vibrational ground state (no excited modes).
- **Fundamentals:** One vibrational quantum is created

$$\prod_{i=1}^{3N-6} \psi_i(0) \rightarrow \left\{ \prod_{i \neq j}^{3N-6} \psi_i(0) \right\} \psi_j(1)$$

— symmetry of vibrational wavefunction determined by the  $j^{\text{th}}$  mode.

## CoL<sub>6</sub> modes in [*trans*-CoCl<sub>2</sub>(en)<sub>2</sub>]<sup>+</sup>

- To understand the electronic spectra of transition metal complexes, it turns out that the vibrational modes have to be considered.
  - Electronic spectrum of [*trans*-CoCl<sub>2</sub>(en)<sub>4</sub>]<sup>+</sup> is shown in Fig. 9.13 in Cotton
- Determine the vibrational modes of the [*trans*-CoCl<sub>2</sub>N<sub>4</sub>] grouping.

## Vibrations of the *trans*-[CoCl<sub>2</sub>N<sub>4</sub>] group

- On p. 293 of Cotton's text *and* on p. 343 of Harris & Bertolucci, the vibrational modes are given as  $2A_{1g}, B_{1g}, B_{2g}, E_g, 2A_{2u}, B_{1u}, 3E_u$

This should be

$2A_{1g}, B_{1g}, B_{2g}, E_g, 2A_{2u}, B_{2u}, 3E_u$

$D_{4h}$	$E$	$2C_4$	$C_2(C_4^2)$	$2C_2'$	$2C_2''$	$i$	$2S_4$	$\sigma_h$	$2\sigma_v$	$2\sigma_d$		
$A_{1g}$	1	1	1	1	1	1	1	1	1	1	$R_z$	$x^2 + y^2, z^2$
$A_{2g}$	1	1	1	-1	-1	1	1	1	-1	-1		
$B_{1g}$	1	-1	1	1	-1	1	-1	1	1	-1		$x^2 - y^2$
$B_{2g}$	1	-1	1	-1	1	1	-1	1	-1	1		$xy$
$E_g$	2	0	-2	0	0	2	0	-2	0	0	$(R_x, R_y)$	$(xz, yz)$
$A_{1u}$	1	1	1	1	1	-1	-1	-1	-1	-1		
$A_{2u}$	1	1	1	-1	-1	-1	-1	-1	1	1	$z$	
$B_{1u}$	1	-1	1	1	-1	-1	1	-1	-1	1		
$B_{2u}$	1	-1	1	-1	1	-1	1	-1	1	-1		
$E_u$	2	0	-2	0	0	-2	0	2	0	0	$(x, y)$	

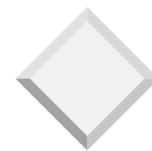
## Example: CO stretching modes for $\text{Cr}(\text{CO})_6$ ( $\text{Mn}(\text{CO})_6^+$ , $\text{V}(\text{CO})_6^-$ )

$O_h$	$E$	$8C_3$	$3C_2$ ( $=C_4^2$ )	$6C_4$	$6C_2$	$i$	$8S_6$	$3\sigma_h$	$6S_4$	$6\sigma_d$		
$A_{1g}$	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
$A_{2g}$	1	1	1	-1	-1	1	1	1	-1	-1		
$E_g$	2	-1	2	0	0	2	-1	2	0	0	$(R_x, R_y, R_z)$	$(2z^2 - x^2 - y^2, x^2 - y^2)$
$T_{1g}$	3	0	-1	1	-1	3	0	-1	1	-1		$(xy, xz, yz)$
$T_{2g}$	3	0	-1	-1	1	3	0	-1	-1	1		
$A_{1u}$	1	1	1	1	1	-1	-1	-1	-1	-1		
$A_{2u}$	1	1	1	-1	-1	-1	-1	-1	1	1		
$E_u$	2	-1	2	0	0	-2	1	-2	0	0		
$T_{1u}$	3	0	-1	1	-1	-3	0	1	-1	1	$(x, y, z)$	
$T_{2u}$	3	0	-1	-1	1	-3	0	1	1	-1		

$\text{Cr}(\text{CO})_6$ :  $A_{1g} \sim 2100 \text{ cm}^{-1}$ ,  $T_{1u} \sim 2000 \text{ cm}^{-1}$ ,  $E_g \sim 1985 \text{ cm}^{-1}$

$\text{Mn}(\text{CO})_6^+$ :  $T_{1u} \sim 2100 \text{ cm}^{-1}$ ,  $\text{V}(\text{CO})_6^-$ :  $T_{1u} \sim 1860 \text{ cm}^{-1}$

Question: What combination and overtone bands are possible?



$O_h$	$E$	$8C_3$	$3C_2$ ( $=C_4^2$ )	$6C_4$	$6C_2$	$i$	$8S_6$	$3\sigma_h$	$6S_4$	$6\sigma_d$		
$A_{1g}$	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
$A_{2g}$	1	1	1	-1	-1	1	1	1	-1	-1		
$E_g$	2	-1	2	0	0	2	-1	2	0	0	$(R_x, R_y, R_z)$	$(2z^2 - x^2 - y^2, x^2 - y^2)$
$T_{1g}$	3	0	-1	1	-1	3	0	-1	1	-1		$(xy, xz, yz)$
$T_{2g}$	3	0	-1	-1	1	3	0	-1	-1	1		
$A_{1u}$	1	1	1	1	1	-1	-1	-1	-1	-1		
$A_{2u}$	1	1	1	-1	-1	-1	-1	-1	1	1		
$E_u$	2	-1	2	0	0	-2	1	-2	0	0		
$T_{1u}$	3	0	-1	1	-1	-3	0	1	-1	1	$(x, y, z)$	
$T_{2u}$	3	0	-1	-1	1	-3	0	1	1	-1		

## Infrared Spectroscopy

Consider  $\int \varphi_j^{gnd} \hat{d} \varphi_j^{exc} d\tau$ ,  
 where  $\hat{d}$  transforms as  $x, y$ , or  $z$

This task is straightforward

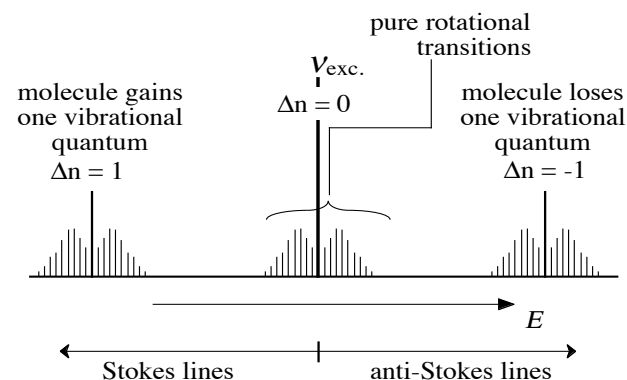
$\Rightarrow$  evaluate  $\Gamma_x \otimes \Gamma_y \otimes \Gamma_z = \Gamma_1$  (totally sym. IR)  
 we know this occurs iff  $\Gamma_x = \Gamma_j$

A Fundamental is infrared active when the excited mode transforms as  $x, y$ , or  $z$ .

## Raman Spectroscopy

- Inelastic scattering of photon (not a resonant absorption spectroscopy)

Example (schematic) - a diatomic molecule in the gas phase



Chandrashekhara  
 Venkata RAMAN  
 1888-1970

## C. V. Raman

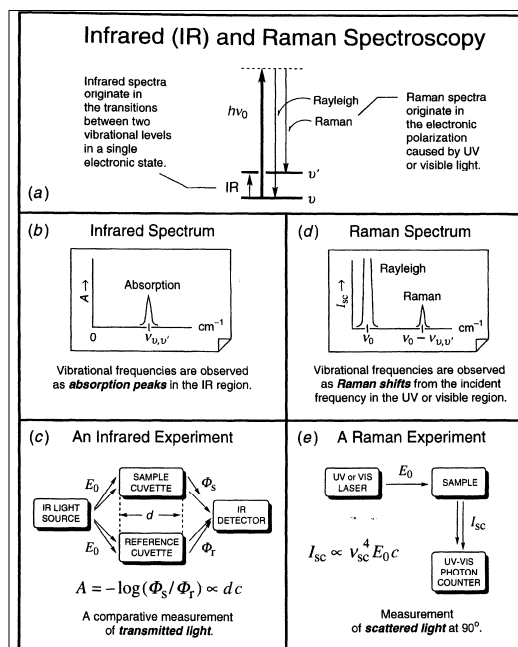
### Nobel Prize in Physics 1930

"for his work on the scattering of light and for the discovery of the effect named after him"

In 1922, Raman published "Molecular Diffraction of Light", first of a series of investigations with his collaborators which ultimately led to his discovery, on the Feb. 28<sup>th</sup>, 1928, of the radiation effect which bears his name ("A new radiation", *Indian J. Phys.*, **2** (1928) 387.)

## IR-Raman Comparison

- IR = absorption; Raman = inelastic scattering
- IR spectrum shows absorption peaks; in Raman vibrational frequencies are observed as shifts from the incident frequency
- in IR an external reference is used for comparison
- in Raman, an intense Rayleigh (elastic scattering) peak is observed with Raman (inelastic) peaks displaced from it - energy difference is absorbed by the molecule
- The exciting radiation must be monochromatic, the signal is proportional to the incident light intensity.



## Polarizability Tensor

$$\begin{bmatrix} d_{x,\text{ind.}} \\ d_{y,\text{ind.}} \\ d_{z,\text{ind.}} \end{bmatrix} = \begin{bmatrix} \alpha_{xx} & \alpha_{xy} & \alpha_{xz} \\ \alpha_{yx} & \alpha_{yy} & \alpha_{yz} \\ \alpha_{zx} & \alpha_{zy} & \alpha_{zz} \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix}$$

Components of the induced dipole created by **E**-field of photon.      Molecular polarizability tensor.      **E**-field of scattering photon.

## Raman Spectroscopy

- Became much more important after development of lasers because only about one thousandth of the scattered radiation is Raman, the rest is scattered elastically (with conservation of energy)
- Selection rules — scattering amplitudes involve the elements of the polarizability tensor (which must be nonzero):

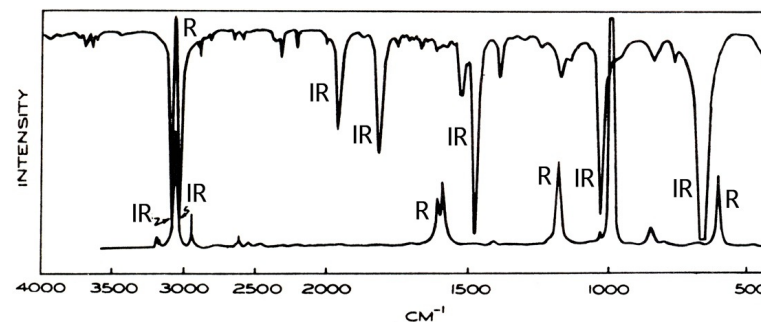
$$\int \psi_j^{\text{gnd}} \alpha_{mn} \psi_j^{\text{exc}} d\tau \sim \Gamma_{mn} \otimes \Gamma_j \quad m, n = x, y, \text{ or } z$$

i.e.,  $\Gamma_j$  must transform as  $x^2, y^2, z^2, xy, xz, yz$

## Exclusion Rule

- If a molecule is centrosymmetric, then allowed infrared transitions are forbidden in the Raman spectrum and allowed Raman transitions are forbidden in the IR. (Why?)
- If an inversion center is present, then  $x, y,$  and  $z$  belong to  $u$  representations and  $\alpha_{mn}$  belong to  $g$  representations.

## Exclusion Rule - Benzene



Vibrational spectra of benzene reproduced from S.K. Freeman, *Applications of Laser Raman Spectroscopy*, John Wiley & Sons, N.Y. 1974.



## Examples

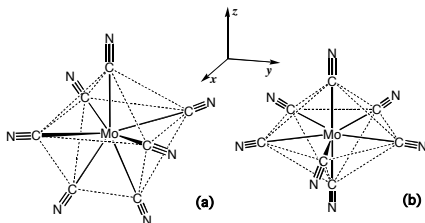
- Describe the number and character of the IR and Raman transitions observed for  $\text{BrF}_5$  if the molecule has  $D_{3h}$  symmetry.  $C_{4v}$  symmetry?
- How can IR and Raman spectra allow one to distinguish between syn- and anti-planar structures of  $\text{N}_2\text{F}_2$ ?
- For  $\text{BF}_3$ , Raman and IR active modes. B-F stretching modes can be observed in both the IR and Raman spectra — which are affected by the presence of two B isotopes ( $^{10}\text{B}$  and  $^{11}\text{B}$ )?

$D_{3h}$	$E$	$2C_3$	$3C_2$	$\sigma_h$	$2S_3$	$3\sigma_v$		
$A_1'$	1	1	1	1	1	1		$x^2 + y^2, z^2$
$A_2'$	1	1	-1	1	1	-1	$R_z$	
$E'$	2	-1	0	2	-1	0	$(x, y)$	$(x^2 - y^2, xy)$
$A_1''$	1	1	1	-1	-1	-1		
$A_2''$	1	1	-1	-1	-1	1	$z$	
$E''$	2	-1	0	-2	1	0	$(R_x, R_y)$	$(xz, yz)$

$C_{4v}$	$E$	$2C_4$	$C_2(C_4^2)$	$2\sigma_v$	$2\sigma_d$		
$A_1$	1	1	1	1	1	$z$	$x^2 + y^2, z^2$
$A_2$	1	1	1	-1	-1	$R_z$	
$B_1$	1	-1	1	1	-1		$x^2 - y^2$
$B_2$	1	-1	1	-1	1		$xy$
$E$	2	0	-2	0	0	$(x, y), (R_x, R_y)$	$(xz, yz)$

## Example

The seven-coordinate complex  $\text{Mo}(\text{CN})_7^{4-}$  has been studied both as solid  $\text{K}_4\text{Mo}(\text{CN})_7 \cdot 2\text{H}_2\text{O}$  and in aqueous solution. In the C—N stretching region the IR spectrum has bands at 2119, 2115, 2090, 2080, 2074, and 2059  $\text{cm}^{-1}$  for the solid and at 2080 and 2040  $\text{cm}^{-1}$  for solutions. How many Raman and infrared bands would you expect for (a) the monocapped trigonal prism and (b) the pentagonal bipyramid and how many coincidences (bands present in both the IR and Raman spectra) should there be for each geometry? How do you interpret these data?



## Fundamentals and Overtones and Combination bands for $\text{XY}_4$ molecules

- On p. 194 of Carter, overtones of  $\text{CH}_4$  are treated incorrectly. Cotton leaves out their treatment entirely. Harris and Bertolucci provide a decent discussion (p. 164-7 and Appendix C).
- Let's work out the normal modes, look at the fundamentals - then discuss how the overtone and combination bands are handled differently

## Overtone - Degenerate Modes; Symmetric Direct Products

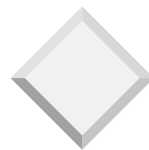
- With two quanta in a degenerate mode, the symmetries of  $\Psi_{vib}$  are given by\*:

$$\chi^+(R) = \frac{1}{2}(\chi^2(R) + \chi(R^2))$$

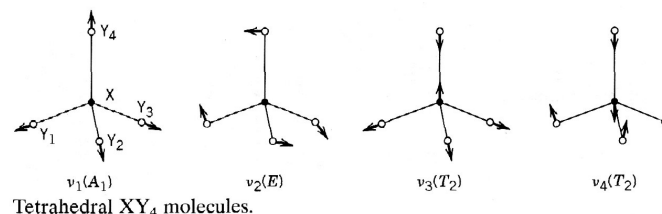
- With three quanta the formula is

$$\chi^+(R) = \frac{1}{6}(\chi^3(R) + 3\chi(R)\chi(R^2) + 2\chi(R^3))$$

(\*See Wilson, Decius, & Cross, "Molecular Vibrations...", Section 7.3; this is the source material for Harris & Bertolucci's Appendix C. Also see the *Antisymmetry* handout for proof for the two and three quanta cases.)



$T_d$	$E$	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
$A_1$	1	1	1	1	1		$x^2 + y^2 + z^2$
$A_2$	1	1	1	-1	-1		$(2z^2 - x^2 - y^2, x^2 - y^2)$
$E$	2	-1	2	0	0	$(R_x, R_y, R_z)$	
$T_1$	3	0	-1	1	-1	$(x, y, z)$	
$T_2$	3	0	-1	-1	1		$(xy, xz, yz)$

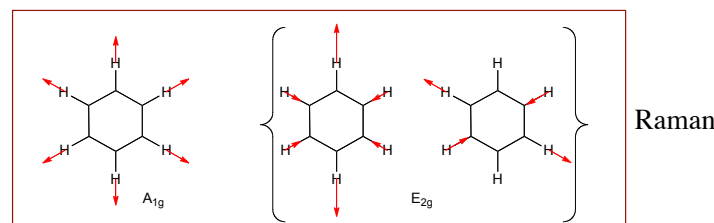


## Fermi Resonance

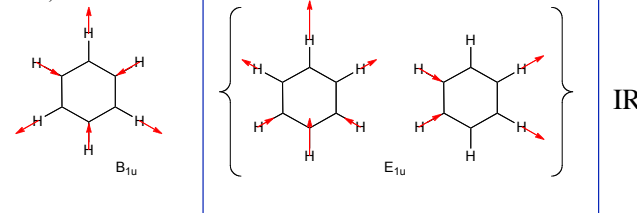
- Just as "configuration interaction" occurs in electronic spectra, mixing between fundamentals and combination or overtone bands can occur in vibrational spectra.
- 'Weak' combination/overtone bands can 'borrow' intensity from fundamentals if the sum of the frequencies in the combination/overtone band is close to the frequency of the fundamental.
- $CO_2$  example from Cotton: fundamental frequencies are 668, 1337 (Raman), 2349  $cm^{-1}$  (what are they?). 200 mixes with 010.

## Example: C-H region of benzene

<http://home.arcor.de/rothw/gauss/varsanyi/molekuele/Bz/>

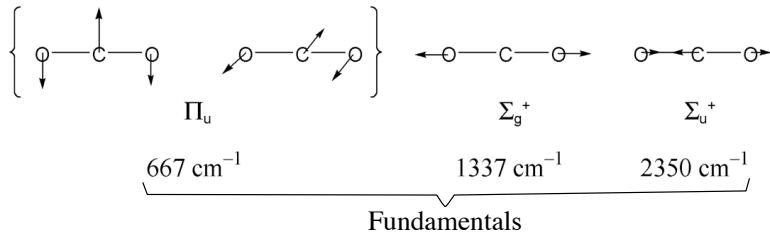
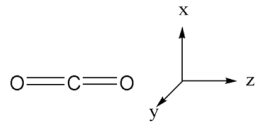


see Wilson, Decius, and Cross



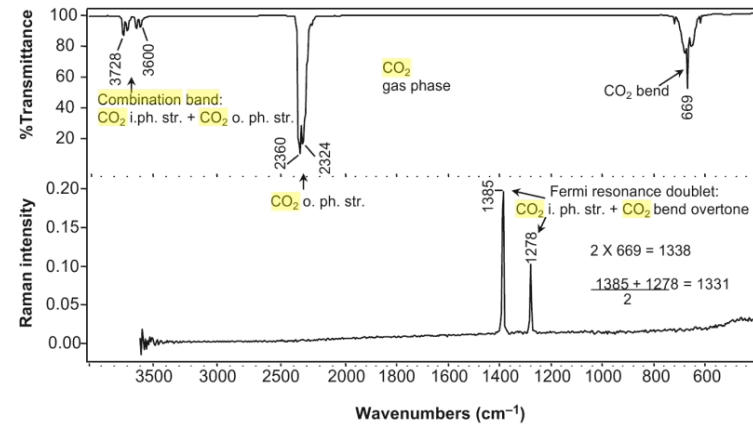
$C_6H_6$ : three IR bands at 3045, 3073, 3099  $cm^{-1}$ ;  $C_6D_6$ : one IR band at 2293  $cm^{-1}$

# Normal Modes and Vibrational Frequencies for CO<sub>2</sub>



Observed Raman bands: 1278 and 1385 cm<sup>-1</sup>

# Vibrational Spectra for CO<sub>2</sub>



Observed Raman bands: 1278 and 1385 cm<sup>-1</sup>

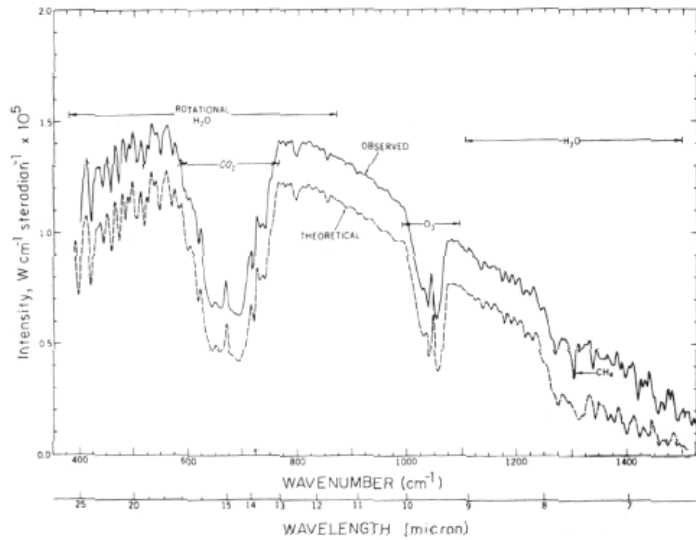


FIG. 6.1. Observed and theoretical spectra for clear skies over the Gulf of Mexico, April 23, 1969. The observed spectrum is displaced upward by  $0.2 \times 10^{-5} \text{ W cm}^{-2} \text{ steradian}^{-1} \text{ wave number}^{-1}$ . After Conrath et al. (1970).

# Planck's Blackbody Radiation Law

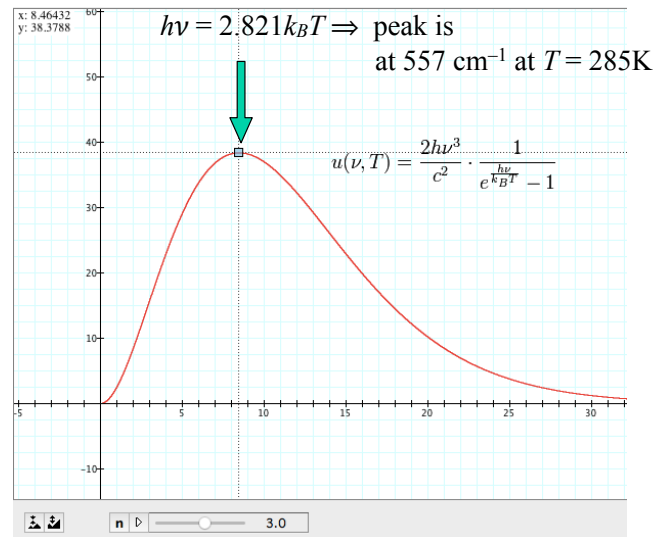


TABLE 4.1 Selected Groups that Display Fermi Resonance Bands in their Vibrational Spectrum.

Group	Bands (cm <sup>-1</sup> )	Assignment	Active	
			IR	Raman
CO <sub>2</sub>	1385, 1278	CO <sub>2</sub> i. ph. str + 2x CO <sub>2</sub> bend	No	Yes
R-C(=O)-H	~2820, ~2710	CH str. + 2x CH i.ph. bend	Yes	Yes
N=C=O <sup>-</sup>	~1300, ~1200	NCO i.ph. str. + 2x NCO bend	Yes	Yes
R-COOH	~3000-2650	OH str. + 2x OH i. pl bend	Yes	Yes
	~3000-2550	OH str. + 2x C-O str.	Yes	Yes
CH <sub>2</sub>	~2920-2890	CH <sub>2</sub> str. + 2 x CH <sub>2</sub> bend	Yes	Yes
Aryl-C(=O)-Cl	~1780, ~1730	C=O str. + 2x 880 aryl-C str.	Yes	Yes
N≡C-N=C(NH <sub>2</sub> ) <sub>2</sub>	2200, 2170	C≡N str. + (1250 + 925 cm <sup>-1</sup> ) Combination band	Yes	-
R-C≡C-R	2300, 2235	C≡C str + C-C≡C bend	No	Yes
C=O	1810, 1780	C=O str. + 2x ~900 ring bend	Yes	-
Aryl-NH <sub>2</sub>	3355, 3205	NH <sub>2</sub> i. ph. str. + 2x NH <sub>2</sub> bend	Yes	Yes
NH <sub>4</sub> Cl	2825	NH <sub>4</sub> i. ph. str. + 2x NH <sub>4</sub> bend	Yes	Yes
-C(=O)-NH-C	3300 (s), 3100(m)	MH str. + 2x CNH str.-bend	Yes	Yes

$D_{\infty h}$	$E$	$2C_{\infty}^{\Phi}$	$\dots$	$\infty\sigma_v$	$i$	$2S_{\infty}^{\Phi}$	$\dots$	$\infty C_2$		
$\Sigma_g^+$	1	1	$\dots$	1	1	1	$\dots$	1		$x^2, y^2, z^2$
$\Sigma_g^-$	1	1	$\dots$	-1	1	1	$\dots$	-1		
$\Pi_g$	2	$2\cos\Phi$	$\dots$	0	2	$-2\cos\Phi$	$\dots$	0	$R_z$	$(xz, yz)$
$\Delta_g$	2	$2\cos 2\Phi$	$\dots$	0	2	$2\cos 2\Phi$	$\dots$	0	$(R_x, R_y)$	$(x^2 - y^2, xy)$
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$		
$\Sigma_u^+$	1	1	$\dots$	-1	-1	-1	$\dots$	1	$z$	
$\Sigma_u^-$	1	-1	$\dots$	-1	-1	1	$\dots$	1		
$\Pi_u$	2	$2\cos\Phi$	$\dots$	0	-2	$2\cos\Phi$	$\dots$	0	$(x, y)$	
$\Delta_u$	2	$2\cos 2\Phi$	$\dots$	0	-2	$-2\cos 2\Phi$	$\dots$	0		
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$		

$$\frac{1}{2}(\chi^2(C^{\Phi}) + \chi(C^{2\Phi})) = \frac{1}{2}(4\cos^2\Phi + 2\cos 2\Phi) = (1 + \cos 2\Phi) + \cos 2\Phi = 1 + 2\cos 2\Phi$$

Therefore,

$$[\Pi_u \otimes \Pi_u]^+ \left| \begin{array}{ccc|ccc} 3 & 1+ & \dots & 1 & 3 & 1+ & \dots & 1 \\ & 2\cos 2\Phi & & & & 2\cos 2\Phi & & \end{array} \right| \Rightarrow \Sigma_g^+ + \Delta_g$$