1. Franck-Condon principle - Electrons make a transition from one electronic state to another so quickly that the nuclei do not move appreciably during the transition.

2. Raman Spectroscopy - Vibration/Rotation involves the electronic polarizability. Must change in vibrations & must be anisotropic for rotations.

3. Coupling of nuclear magnetic moments & electron spin.

4. In Raman spectroscopy, the incident photons may increase in energy (anti-Stokes) or decrease in energy (Stokes). Stokes lines appear at frequencies lower than the incident photons while anti-Stokes are higher.

5. If a diatomic molecule is in a vibrational energy level with energy $E_v$ and is moving in the potential $V(R)$ where $R$ is the bond length, then the classical turning points ($R_{\pm}$) are those for which $V(R_{\pm}) = E_v$. 
6. $^3\Sigma_g^-, \Delta_g \to ^1\Sigma_g^+$

7. $N+1$ lines with a binomial intensity distribution

8. Fluorescence - radiative decay (transitions) between two states of the same spin multiplicity.

Phosphorescence - radiative transition between two states of different spin multiplicity

Intersystem crossing - non radiative decay between two states of different multiplicity.

Internal Conversion - non radiative decay between states of the same multiplicity.

9. $\chi = \frac{d^2V}{dx^2} + 2\beta^2D_e$ (work through details!)

10. $\hat{H} = \hat{H}^0 + \hat{H}'$; $\hat{H}^0 = Hamiltonian$ in absence of radiation field.

$\hat{H}' = -\vec{\mu} \cdot \vec{E}$; coupling to field; $\vec{\mu} = dipole$ moment

$\vec{E} = E \cos \omega t$

Time dependent Schrödinger equation $\frac{d}{dt}\Psi(x,t) = -\frac{i}{\hbar} \frac{\partial \Psi}{\partial t}$

Use ansatz $\Psi = a_1(t) \Psi_1^0(x,t) + a_2(t) \Psi_2^0(x,t)$

$\hat{H}^0 \Psi^0 = -\frac{\hbar}{i} \frac{\partial \Psi^0}{\partial t}$
Insert $\Psi$ into the Schrödinger Equation, multiply by $\frac{\hbar}{2} \Psi^*$ and integrate. Boundary conditions $A_1(0)=1$, $A_2(0)=0$. Assume $A_1(t) \approx 1$ and solve for $\frac{dA_2}{dt}$.

This results in $A_2(t) \approx \mu_{21} \, E^* \sin \left( \frac{\omega - \omega_{21}}{\hbar} t \right)$

where $\omega_{21} = \omega_2 - \omega_1 = (E_2^* - E_1^*) / \hbar$

$\mu_{21} = \langle 2| x | 1 \rangle$ & this is not zero if $2 \neq 1$

differ by 1 vibrational quantum.

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H $c$ $c$
H $c$ $c$

4 atoms :: 6 vibrations

Trans $\quad$ Rot

$A_{A_1} = \frac{1}{4} \left( 12 - 2 + 2 + 4 \right) = 4$ $3$ $\quad$ $-$$R_3$

$A_{A_2} = \frac{1}{4} \left( 12 - 2 - 2 - 4 \right) = 1$ $-$$R_3$

$A_{B_1} = \frac{1}{4} \left( 12 + 2 + 2 - 4 \right) = 3$ $X$$R_Y$

$A_{B_2} = \frac{1}{4} \left( 12 + 2 - 2 + 4 \right) = 4$ $Y$$R_X$

$\Gamma_{vib} = 3A_1 + B_1 + 2B_2$ & all are IR &

\begin{align*}
\text{Raman active}
\end{align*}