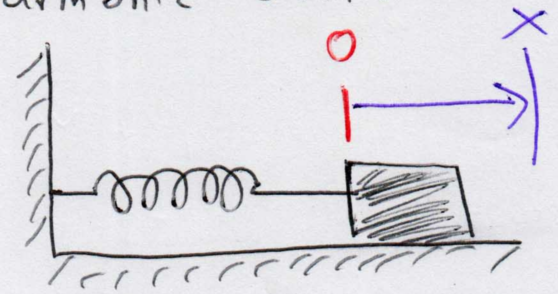
5/22/12

Harmonic Oscillator



Force → $F = -kx$ ← spring constant

$m \cdot a = -kx$

$a = \Delta v / \Delta T$

$v = \Delta x / \Delta T$

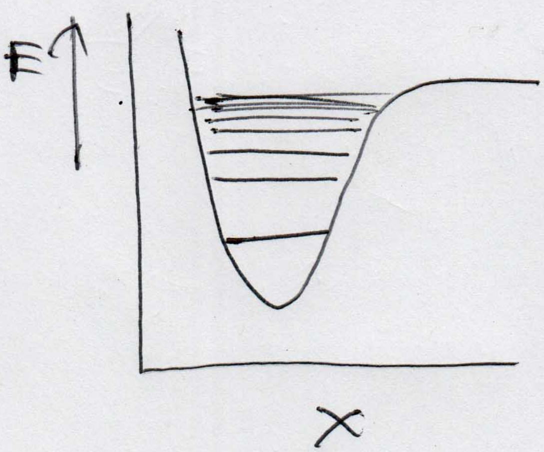
$a = \Delta(\Delta x / \Delta T)$

$$m \cdot \frac{\partial^2 x}{dt^2} = -kx$$

$f(x) = e^{ix}$

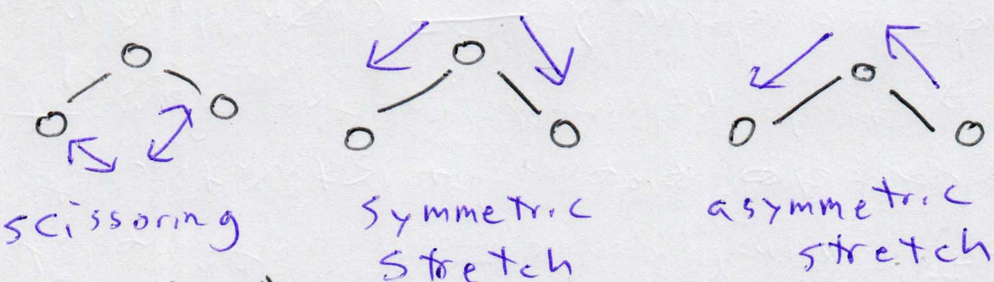
$f(x) = \sin \omega x$

The harmonic oscillator reasonably describes the motion of two atoms in a bond.

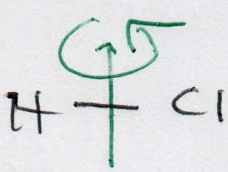


Since energy at the atomic level is quantized (only comes in discreet packets), there are only specific vibrational energy levels available to a bond.

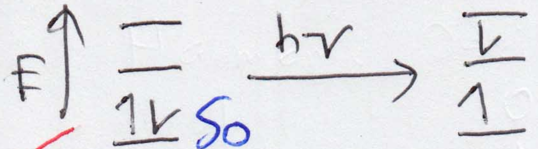
Modes of vibration



Rotational energy levels



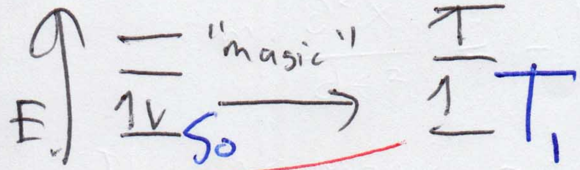
Rotational motion is also quantized @ the atomic level, so only specific rotational energy levels can exist for a system.



When an electron is excited between energy levels, the spin of the electron must be maintained (a spin-allowed transition)

ground state → total spin = 0

$m = 2 \cdot 0 + 1 = 1$ ← singlet

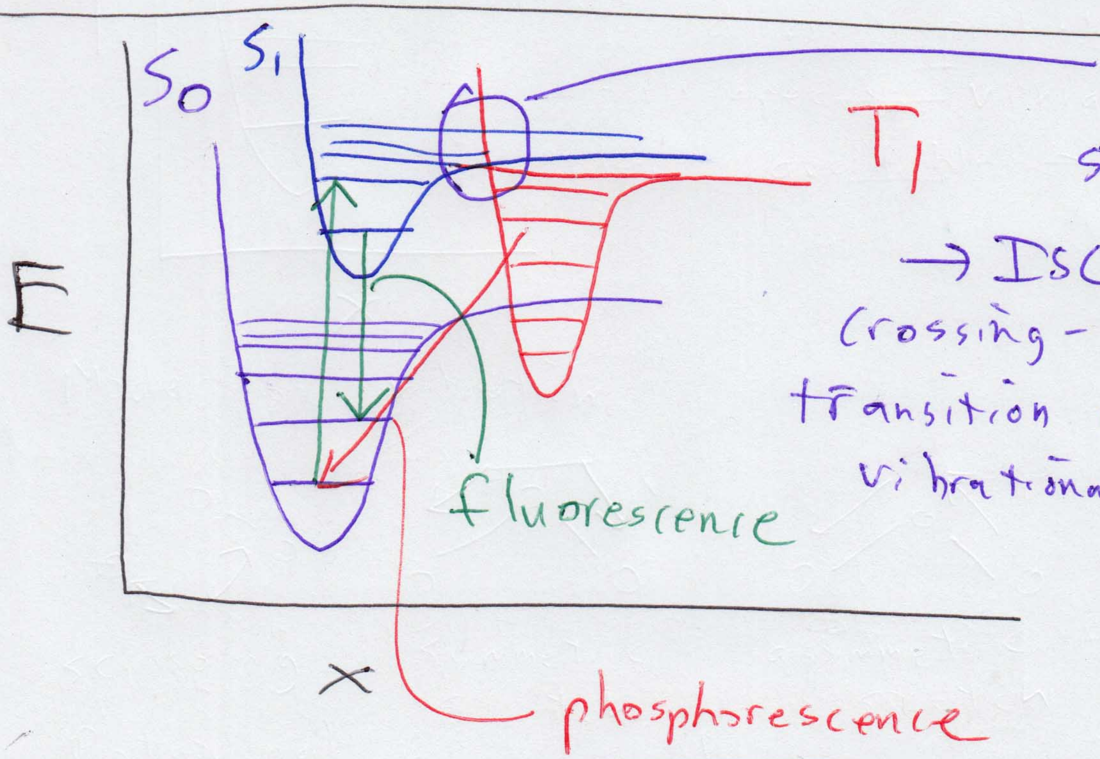


If a spin flips during transition between energy levels, it is called a spin-forbidden transition, since it is technically not possible.

→ total spin = 1

$m = 2 \cdot 1 + 1 = 3$ ← triplet

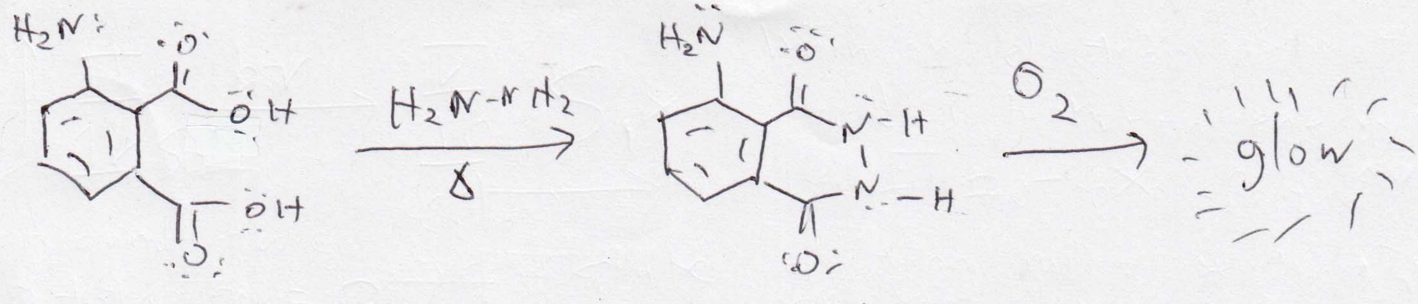
spin multiplicity: $m = 2S + 1$
total spin ↗



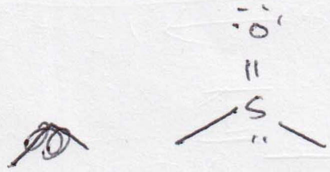
vibrational states match

→ ISC - inter-system crossing - a spin-forbidden transition enabled due to vibrational states

Chemilluminescence - A phenomenon caused by a chemical reaction ~~that~~ in which the reaction itself causes the formation of an excited state intermediate that then can ~~[illegible]~~ relax to the ground state radiatively (by releasing light).



luminol



DMSO