Selection rule of a rigid diatomic molecule for obtaining a rotational spectrum.

(A rotating molecule having a permanent dipole or generates an electric field which can interact with the electric component of the microwave region.)

If it is assumed that a diatomic molecule behaves like a rigid rotator, the rotational energy levels may be calculated by solving the Schrodinger's equation.

$$E_J = \frac{h^2}{8\pi^2 I} J(J+1) \text{ Joules where } J = 0, 1, 2.$$

h - Planck's constant

I - Moment of Inertia.

J - Rotational quantum no.

In rotational region, spectra are generally expressed interms of wave numbers, so it becomes useful to consider energies in these units.

$$\therefore \bar{\nu} = \frac{\Delta E_J}{hc} = \frac{h^2}{8\pi^2 I hc} [J(J+1) - J'(J'+1)].$$

$$= \frac{h}{8\pi^2 I c} [J(J+1) - J'(J'+1)].$$

$$= B [J(J+1) - J'(J'+1)].$$

B - rotational constant

When $J = 1$, $J' = 0$ the above eqn. becomes

$$\bar{\nu}_{J_0 \to 1} = B[(1+1) - 0(0+1)]$$

$$= 2B \ cm^{-1}$$ J' = lower level

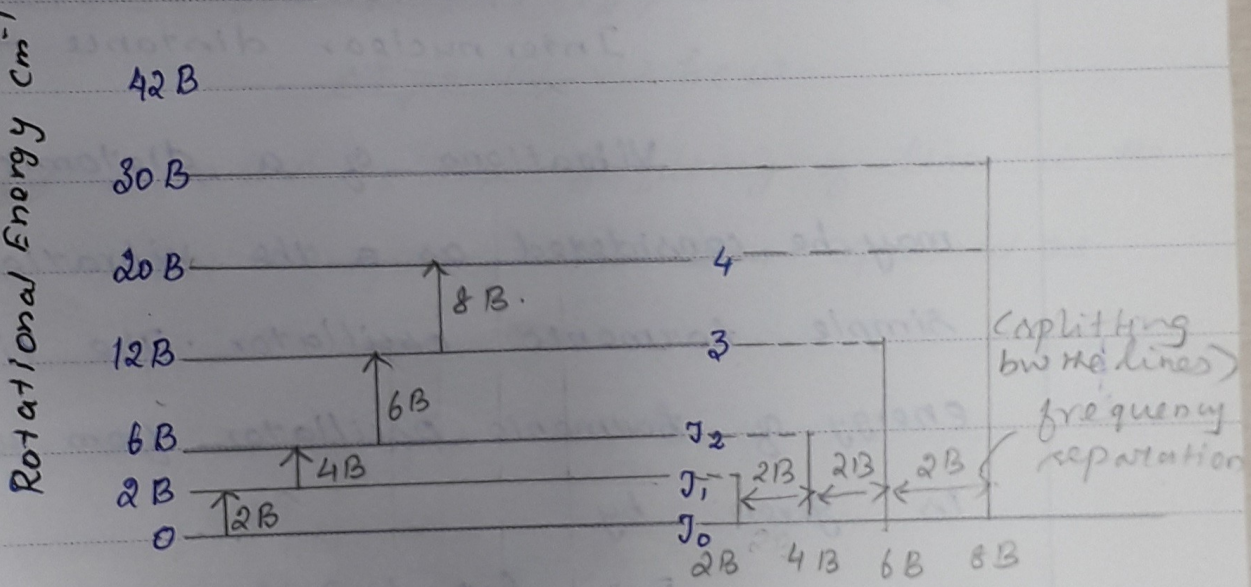
When $J = 2$ to $J' = 1$

$$\bar{\nu}_{J_1 \to 2} = B[2(2+1) - 1(1+1)]$$

$$= B(6-2) = 4B \ cm^{-1}$$

In general, when the molecule is raised from J to $J+1$ the eqn. becomes,

$$\bar{\nu}_{J \to J+1} = 2B(J+1) \ cm^{-1}.$$



Rotational Spectrum of a rigid diatomic molecule.