Answer on the question #65950, Chemistry / Other

Question:

Using a suitable diagram, discuss the rotational spectrum of a rigid diatomic molecule.

Answer:

Spectroscopic lines always correspond to transitions between energy levels. Like electronic spectral lines are the transitions between electronic energy levels, rotational spectral lines are the transitions between rotational energy levels.

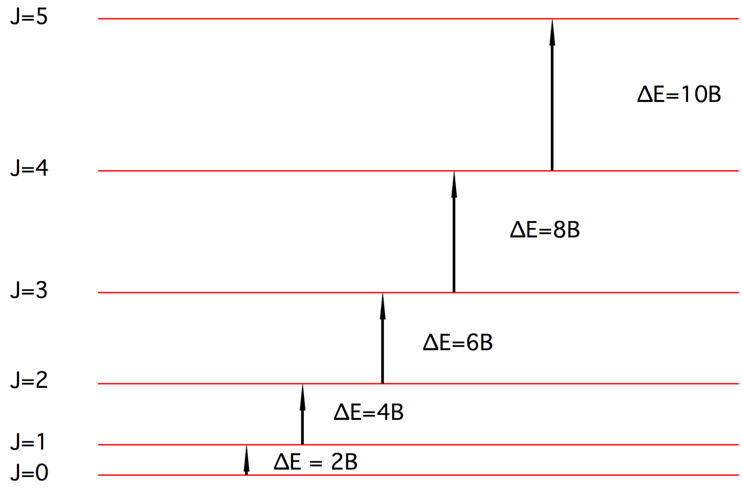

Figure 1. Diagram of rotational energy levels of a molecule. Transitions are showed from lower to higher energy level, assigned to absorption spectra.

Fig. 1 shows the energy diagram and transitions between rotational energy levels. Each rotational energy level corresponds to some quantum number J, giving the energy:

$$E_J = BJ(J+1).$$

As one can notice, transitions are allowed only with the $\Delta J = 1$. Also, the difference between the rotational energy levels is linked to rotational constant B:

$$B = \frac{\hbar}{2I},$$

where I is the inertia moment of the molecule. For diatomic molecule, we get the following expression:

$$I = \mu l^2 = \frac{M_1 M_2}{M_1 + M_2} l^2,$$

where l is the distance between the atoms, μ is reduced mass, M_1 and M_2 are the masses of the first and second atom.

Hence, one can make a conclusion that the spectrum in frequency scale will consist of a series of equally separated lines (2B).