16.5 The rotational energy levels

The rotational energy levels of a rigid rotor may be obtained by solvi Schrödinger equation. Fortunately, however, there is a much less onerc exact expressions that depends on noting the classical expression fc rotating body, expressing it in terms of the angular momentum, and quantum mechanical properties of angular momentum into the equati

The classical expression for the energy of a body rotating about an

$$E_a = \tfrac{1}{2} I_a \omega_a^2$$

where ω_a is the angular velocity (in radians per second, rad s^{-1}) about tl corresponding moment of inertia. A body free to rotate about three

$$E = \tfrac{1}{2} I_a \omega_a^2 + \tfrac{1}{2} I_b \omega_b^2 + \tfrac{1}{2} I_c \omega_c^2$$

Because the classical angular momentum about the axis a is $J_a =$ expressions for the other axes, it follows that

$$E = \frac{J_a^2}{2I_a} + \frac{J_b^2}{2I_b} + \frac{J_c^2}{2I_c}$$

This is the key equation. We described the quantum mechanical pr momentum in Section 12.7b, and can now make use of them in co equation to obtain the rotational energy levels.

$E_J = J(J+1)\,hcB$

(a) Spherical rotors

When all three momenta of inertia are equal to some value I, as in CH_4 a expression for the energy is

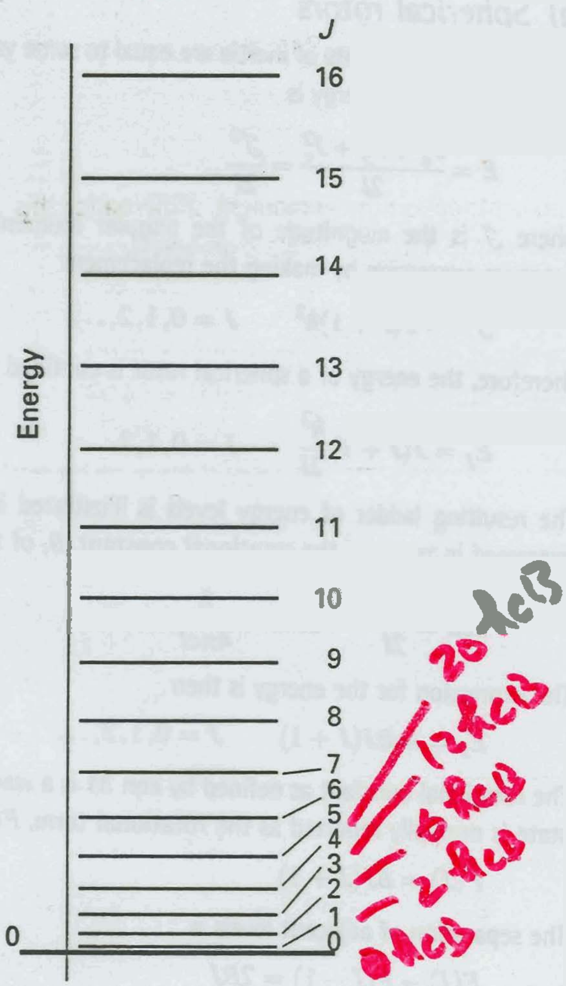
$$E = \frac{J_a^2 + J_b^2 + J_c^2}{2I} = \frac{\mathcal{J}^2}{2I}$$

where $\mathcal{J}$ is the magnitude of the angular momentum. We can im quantum expression by making the replacement

$$\mathcal{J}^2 \rightarrow J(J+1)\hbar^2 \qquad J = 0, 1, 2, \ldots$$

Therefore, the energy of a spherical rotor is confined to the values

$$E_J = J(J+1)\frac{\hbar^2}{2I} \qquad J = 0, 1, 2, \ldots$$



16.17 The rotational energy levels of a linear or spherical rotor. Note that the energy separation between neighbouring levels increases as J

The resulting ladder of energy levels is illustrated in Fig. 16.17. The expressed in terms of the rotational constant, B, of the molecule, wh

$$hcB = \frac{\hbar^2}{2I} \qquad \text{so } B = \frac{\hbar}{4\pi c I}$$

The expression for the energy is then

$$E_J = hcBJ(J+1) \qquad J = 0, 1, 2, \ldots$$

The rotational constant as defined by eqn 31 is a wavenumber.[6] The er state is normally reported as the rotational term, $F(J)$, a wavenumbe

$$F(J) = BJ(J+1)$$

The separation of adjacent levels is

$$F(J) - F(J-1) = 2BJ$$

6 The definition of B as a wavenumber is convenient when we come to vibration–rotation spectra. Ho