Calculate the energies of the first four rotational levels of HI, R = 160pm, allowing it to rotate in three dimensions about its center of mass. Express the answer in J and KJ per mole.

Solution) HI is a diatomic molecule and the rotational spectrum of a diatomic molecule consists of a series of equally spaced absorption lines, typically in the microwave region of the electromagnetic spectrum.

Now energy of rotational levels is given by

$E = J(J+1)\hbar^2/2I$

Here I = moment of inertia of the molecule given by

$I = m_1 m_2 R^2/(m_1 + m_2)$

Here m_1 = mass of Hydrogen atom = 1amu

m_2 = mass of Iodine atom = 127 amu

$R = 160pm = 160 \times 10^{-12}$ m

Thus $I = 1*127\ (160 \times 10^{-12})^2 / (1 + 127)$

Or $I = 25400 \times 10^{-24} = 2.54 \times 10^{-20}$

$\hbar = 1.054 \times 10^{-34}$ J.s

Thus $\hbar^2/2I = 0.2188 \times 10^{-48}$

Thus the energies of first four rotational levels are calculated as below

a) For first energy level J = 1
Or $E = 1*2*\hbar^2/2I = 2 * 0.2188 \times 10^{-48} = 0.4376 \times 10^{-48}$ Joules
Also $E = 0.4376 \times 10^{-48} \times 6.023 \times 10^{23}$ J/mole
$E = 2.635 \times 10^{-25}$ J/mole

b) For first energy level J = 2
$E = 2*3*\hbar^2/2I = 1.312 \times 10^{-48}$ Joules
Also $E = 1.312 \times 10^{-48} \times 6.023 \times 10^{23}$ J/mole $= 7.905 \times 10^{-25}$ J/mole

c) For first energy level J = 3
$E = 3*4*\hbar^2/2I = 2.6256 \times 10^{-48}$ Joules
Also $E = 2.6256 \times 10^{-48} \times 6.023 \times 10^{23}$ J/mole $= 15.81 \times 10^{-25}$ J/mole

d) For first energy level J = 4

$E = 4*5*\hbar^2/2I = 4.376 \times 10^{-48}$ Joules

Also $E = 4.376 \times 10^{-48} \times 6.023 \times 10^{23}$ J/mole $= 26.35 \times 10^{-25}$ J/mole