1 Problem 1

The rotational constant, B_e, for IBr determined from microwave spectroscopy is 0.2241619 cm^{-1}. Approximate the bond length of this molecule.

1.1 Solution

From the Handbook:

$$B_e = \frac{h}{8\ \pi^2\ \mu\ R_e^2}$$

Rearranging gives the required form for solving for the equilibrium bond length of the molecule:

$$R_e = \sqrt{\frac{h}{8\ \pi^2\ \mu\ B_e}}$$

2 Problem 2

How would you compute the energy change associated with a rotation-vibration transition of a diatomic molecule from n=0 to n=1, and J=1 to J=2, using as many corrections to the rotational and vibrational energetics of the molecule. Provide the solution in terms of wavenumbers. Recall that $\omega_e = 2\ \pi\ \nu$, where ν is in the units of sec^{-1}.

2.1 Solution

The energy for a given vibrational state, n, and rotational state, J, is given by (considering the higher corrections for anharmonicity, centrifugal distortion, and vibration-rotation coupling:

$$E = -D_e + \left(n + \frac{1}{2}\right) \hbar\ \omega_e - \left(n + \frac{1}{2}\right) \hbar\ x_e\ \omega_e + h\ B_n\ J\,(J+1) - h\ D_c\ J^2\ (J+1)^2$$

Compute the above expression for the two states given. This gives the energy in convenional units. To convert to wavenumbers, we divide by $h\ c$, where c is the speed of light.