

VIBRATIONAL STATES IN A DIATOMIC MOLECULE (HCL)

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 5.3.

A diatomic molecule such as HCl has a vibrational energy, in which the two atoms can be thought of as connected by a spring with a spring constant k . From basic (non-quantum) physics, the oscillation frequency ω of two masses connected by a spring is

$$(1) \quad \omega = \sqrt{\frac{k}{\mu}}$$

where μ is the reduced mass

$$(2) \quad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

Chlorine has two stable isotopes: Cl^{35} and Cl^{37} . If we take the mass of each atom as the number of nucleons (protons and neutrons) multiplied by the proton weight (not strictly accurate, but pretty close), then the reduced mass of HCl in the two cases is

$$(3) \quad \mu_{35} = \frac{35}{36} m_p$$

$$(4) \quad \mu_{37} = \frac{37}{38} m_p$$

The quantum energy of a harmonic oscillator is

$$(5) \quad E_n = \left(n + \frac{1}{2} \right) \hbar \omega$$

and the energy of a photon produced by a transition between two adjacent energy levels is therefore

$$(6) \quad \Delta E = \hbar \omega = h\nu$$

where ν is the frequency of the photon. The difference in frequency due to the two isotopes is therefore proportional to the difference in the oscillator frequency, so we get

$$(7) \quad \frac{\Delta\nu}{\nu} = \frac{\Delta\omega}{\omega}$$
$$(8) \quad = \left(\frac{1}{\sqrt{\mu_{35}}} - \frac{1}{\sqrt{\mu_{37}}} \right) \sqrt{\mu}$$

For μ we can take an average chlorine mass, so we can take $\mu = \frac{36}{37}m_p$. Plugging in the numbers, we get

$$(9) \quad \frac{\Delta\nu}{\nu} = 7.513 \times 10^{-4}$$