Calculation of a Vibrational Frequency for the C-Cl Bond

We start with our fundamental equation for calculating frequencies,

\[ \nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \]

Where \( k \) is the molecular force constant and \( \mu \) is the reduced mass given by the following equation,

\[ \mu = \frac{m_1 \cdot m_2}{m_1 + m_2} \]

The unit of reduced mass needs clarification. The result of this calculation gives us atomic mass units, or amu. Essentially this means that we are actually calculating the mass of a single molecule made up of two atoms. To work in our equation, we must have units of mass, that is, kilograms (kg) so we must convert the reduced mass units (amu) to kilograms (kg). The simplest way to do this is to multiply by a conversion factor, \( 1.66 \times 10^{-27} \text{ kg/amu} \).

In addition, the unit given for the force constant is “okay” but since we are using SI units, we must convert it to Newtons/meter, and this is just a division by 1000. So rather than use 500,000 ergs/cm\(^2\), we will use 500 N/m (500 kg/sec\(^2\)).

For a C-Cl bond we would put the following into our equation,

\[ \nu = \frac{1}{2\pi} \sqrt{\frac{500 \text{ kg/sec}^2}{\frac{12 \text{ amu} \cdot 35.45 \text{ amu}}{12 \text{ amu} + 35.45 \text{ amu}} \cdot 1.66 \times 10^{-27} \text{ kg/amu}}} \]

\[ \nu = 2.917 \times 10^{13} \text{ sec}^{-1} \]

Okay, but this is not what we really want. The units are wrong. We want wavenumbers, or cm\(^{-1}\). If we remember that \( c = \lambda \nu \), (and use \( c = 3 \times 10^{10} \text{ cm/sec} \) rather than \( 3 \times 10^8 \text{ m/sec} \)) we can solve for \( \lambda \), or more specifically, \( 1/\lambda \),

\[ \frac{1}{\lambda} = \frac{\nu}{c} = \frac{2.917 \times 10^{13} \text{ sec}^{-1}}{3 \times 10^{10} \frac{\text{cm}}{\text{sec}}} = 972.4 \frac{1}{\text{cm}} \]

So, we would expect this bond to be found at 972 wavenumbers on an IR spectrum (assuming that the force constant is 500 N/m).