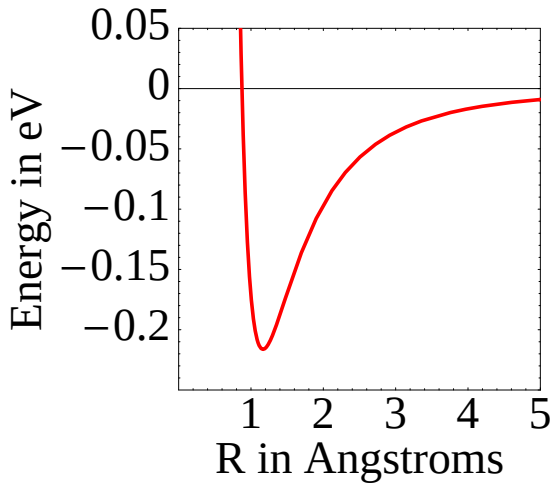
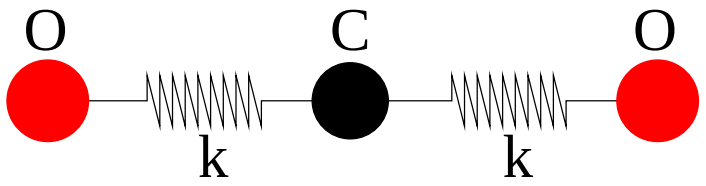
Molecular Vibrations

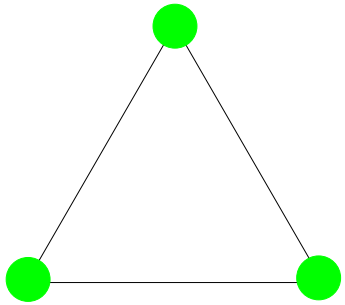
Our picture of the interactions of atoms within a molecule is often built on classical ideas. The motion of atoms in a CO_2 molecule can be described as point particles attached by springs. The spring constant for the $\mathrm{C}-\mathrm{O}$ bond is $7.0\ eV/\mathring{A}^2$ derived from the bond potential shown below. Suppose our 'toy' CO_2 molecule is 'plucked' by pulling the left-hand-side oxygen atom $0.2\ \mathring{A}$ to the left and the right-hand-side oxygen $0.2\ \mathring{A}$ to the right. Both atoms are then released from rest. What is the position of each atom in the molecule as a function of time?





More Molecular Vibrations

Consider a ‘classical’ model of a molecule like cyclopropane, $\mathrm{C_3H_6}$ shown below. The equations of motion are shown below.



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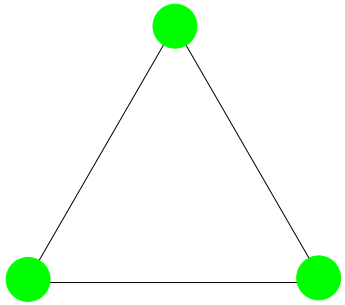

$$\ddot{x}_1 + \tfrac{1}{4}\omega_0^2\left[5x_1 - 4x_2 - x_3 + \sqrt{3}(y_1 - y_3)\right] = 0$$

$$\ddot{x}_2 + \tfrac{1}{4}\omega_0^2\left[-4x_1 + 5x_2 - x_3 + \sqrt{3}(y_3 - y_2)\right] = 0$$

$$\ddot{x}_3 + \tfrac{1}{4}\omega_0^2\left[-x_1 - x_2 + 2x_3 + \sqrt{3}(y_2 - y_1)\right] = 0$$

$$\ddot{y}_1 + \tfrac{1}{4}\omega_0^2\left[\sqrt{3}(x_1 - x_3) + \sqrt{3}(y_1 - y_3)\right] = 0$$

$$\ddot{y}_2 + \tfrac{1}{4}\omega_0^2\left[\sqrt{3}(x_3 - x_2) + \sqrt{3}(y_2 - y_3)\right] = 0$$

$$\ddot{y}_3 + \tfrac{1}{4}\omega_0^2\left[\sqrt{3}(x_2 - x_1) + \sqrt{3}(-y_1 - y_2 + 2y_3)\right] = 0$$