

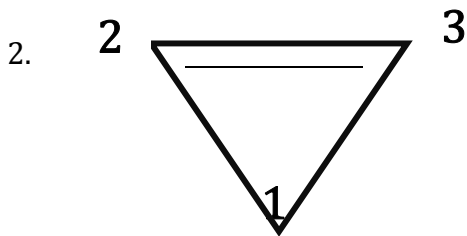
Chem 2430 HW #7

1. The Morse potential is defined as $V(r) = D_e \left(1 - e^{-a(r-r_e)}\right)^2$ where D_e is the dissociation energy and r_e is the equilibrium bond length.

Expand the potential in powers of $(r - r_e)$, keeping terms up to the fourth order.

Show that the force constant $k = 2D_e a^2$

What is the value of the anharmonicity constant $\omega_e x_e$? (Note this utilizes an earlier homework result.)



Consider the C_3H_3 cyclopropenyl radical, with the C atoms numbered 1,2,3, as shown in the figure. For this problem the Huckel energies are $\alpha + 2\beta$, $\alpha - \beta$, $\alpha - \beta$.

Suppose $\alpha = -5\text{eV}$, $\beta = -4\text{eV}$.

Now change the CH group in position 1 to an N atom, with an assumed α value of -5.5 eV. How are the energies of the three π orbitals shifted by this substitution?

3. Consider two coupled oscillators with the potential given by

$$\frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2 + \frac{q^2x_1x_2}{R^3}$$

where R is the fixed separation between the oscillators.

Note $(qx_1)(qx_2)/R^3$ represents the coupling of two dipoles. Show that the potential can be separated by a change of variables.

What is the change of the zero-point energy caused by the coupling term?

You can also treat this problem using second order perturbation theory. In that approach, what is the energy change due to the coupling?