Chemistry 531 Problem Set 7

Due 12/8/00

1. Homework assigned in the Normal Mode Analysis "Handout".

2. Diagonalize the force constant matrix for a model of linear CO_2, given by the following potential in mass-scaled cartesian coordinates.

$$V = \frac{1}{2}k_1(x_{CO} - x_{CO}^e)^2 + \frac{1}{2}k_1(x_{CO'} - x_{CO'}^e)^2 + 2*\frac{1}{2}k_{12}(x_{CO} - x_{CO}^e)(x_{CO'} - x_{CO'}^e)$$

O----------C---------O -----> x-axis

Determine the normal coordinates and the normal mode frequencies andsketch the normal modes. One is termed the "symmetric stretch" and the other is termed the "antisymmetric stretch". Given that ω_1 = 1350 cm^{-1} and ω_2 = 2400 cm^{-1}, work backwards to determine k_1 and k_{12}. Report their values in hartrees/(atomic units of mass scaled*length)

3. Given the following cartesian coordinates, locate the center of mass of the molecule (HOCO). Then determine the intertia tensor with respect to the center of mass.

x	y	z	Atom
2.80	0.0	0.0	O (15.9949146)
0.0	0.0	0.0	C (12.0)
-1.3270	-1.7547	0.0	O (15.9949146)
3.9129	1.6012	0.0	H (1.007825035)