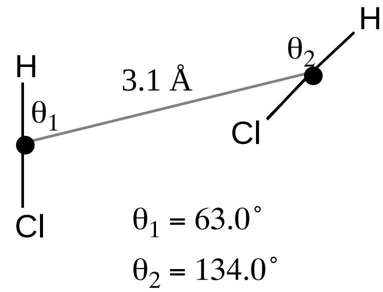
Take-Home Examination 1 **October 8, 1996**

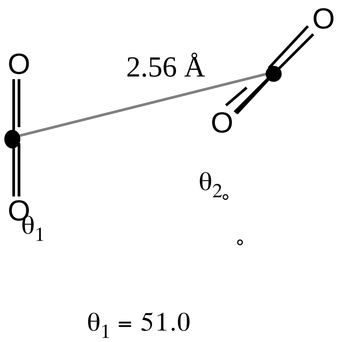
Chemistry 262 **Dr. Jay H. Baltisberger**

Name: ________________________

Please answer all 6 questions, showing all calculations - 12 points each, 72 total.

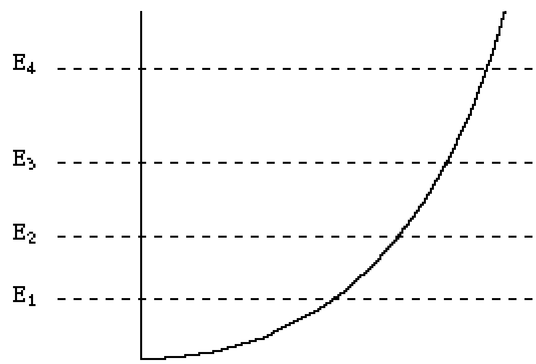
1. Calculate the dipole moment for an HCl molecule as well as the energy of interaction between two HCl molecules with bond distance 1.2 Å using the dipole/dipole model (assuming the Cl has a –0.4 charge while the H a +0.4 charge) with the geometry given in the figure to the right.





2. Calculate the energy of interaction for a pair of oxygen molecules (assuming a 1.4 Å bond length) which in the geometry given in the figure to the left. Use the London-van der Waals interaction using constants given in table 9.1. Note in both this problem and the previous one, geometry is critical to the solution. Think about where the atoms are relative to one another!

3. Draw (graphically, indicating how the wavelength will change) the 4 lowest energy wavefunctions for a particle in a one-dimensional box with the potential energy given in the figure to the right. Note the E_1 through E_4 denote the energies of the first four energy levels in this particular box. Also the left and right walls are infinite boundaries.



4. Assume that a molecule, $PtCl_4$ is described by a two-dimensional particle in a box hamiltonian. Calculate the energy for the lowest energy transition if the molecule is considered square planar with sides of 5.0 Å and the total number of electrons in the box is only the valence electrons of chlorine.

5. What is the probability of finding a single electron in the region from 1.0 to 1.5 Å in a 3.0 Å wide one dimensional box if the electron is in the 4th excited state (n = 5).

6. If the wavefunction for the harmonic oscillator ground state was approximated as $\Psi_0(x) = A \cos(\pi x) \exp(-x^2)$ for a particle with $k = 2$, $m = 2$ and A an arbitrary normalization constant. Calculate the wavefunction for the first excited state, $\Psi_1(x)$. Note that this requires using the operators to calculate a new wavefunction from the equation $\Psi_1(x) = \mathbf{a}^\dagger\ \Psi_0(x) / C_0$ where operators and coefficents take usual definitions.