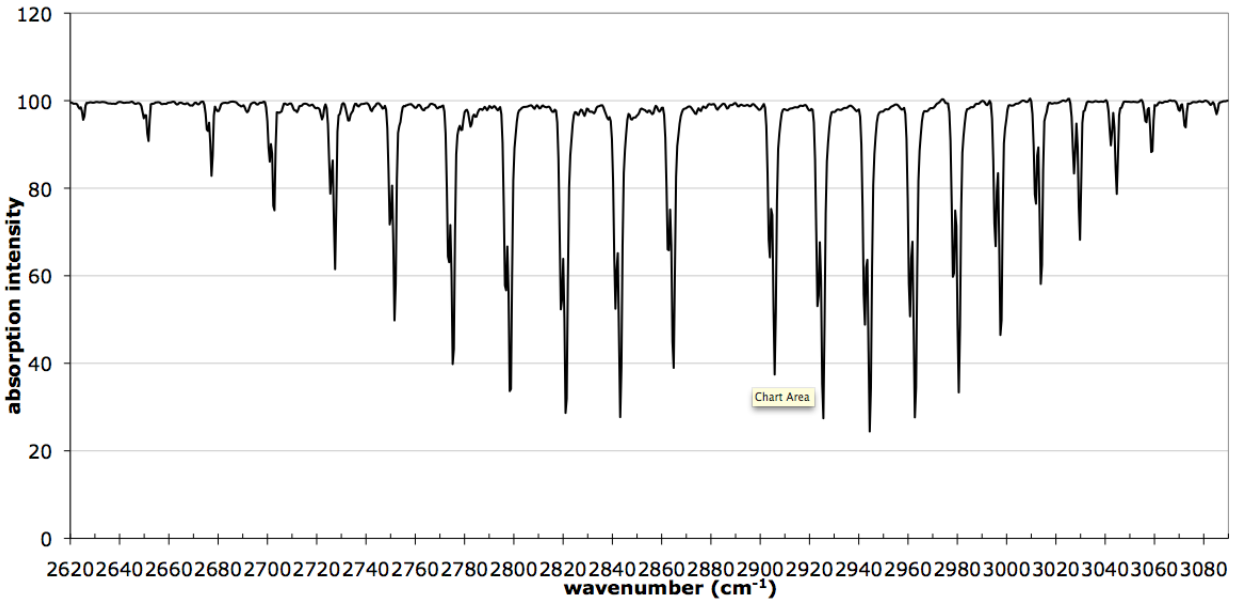
Creighton University Professor G. Duda
Physics 531: Quantum Mechanics Fall 2013

Project #4: Rotational-Vibrational Spectroscopy of HCl

In this next project we're going to examine the energy levels of a realistic system that we can model with our understanding of quantum mechanics. The HCl molecule has several degrees of freedom: it of course has the usual three translational degrees of freedom, but it addition to these, HCl can also oscillate like a spring or rotate like a rigid rotor adding two extra degrees of freedom.

Below is a FTIR spectroscopy image of the absorption spectrum of HCl.



The main objectives for this project include the following:

1. To model this system quantum mechanically by writing down a Hamiltonian and finding the wave functions of the energy eigenstates and the allowed energies both through algebraic methods and through solving the Schrodinger equation (series solutions method).

2. To derive the selection rules for this system in order to understand which rotational and vibrational transitions are allowed.

3. To use our theoretical machinery to predict and explain the spectrum above.

4. To compare our theoretical results to data and by doing so determine the bond length and moment of inertia of HCl.