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### Ultra-high vibrational and rotational motion of the HF molecule via Infrared (IR) laser excitation

Toria Tucker  
*DePauw University*

Jingwei (Mike) Ling  
*DePauw University*

Bridget Gourley  
*DePauw University*

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# Theoretical prediction of ultrahigh vibrational excitation using infrared picosecond pulse trains

Jingwei Ling\*, Toria Tucker\*, and Bridget L. Gourley, PhD

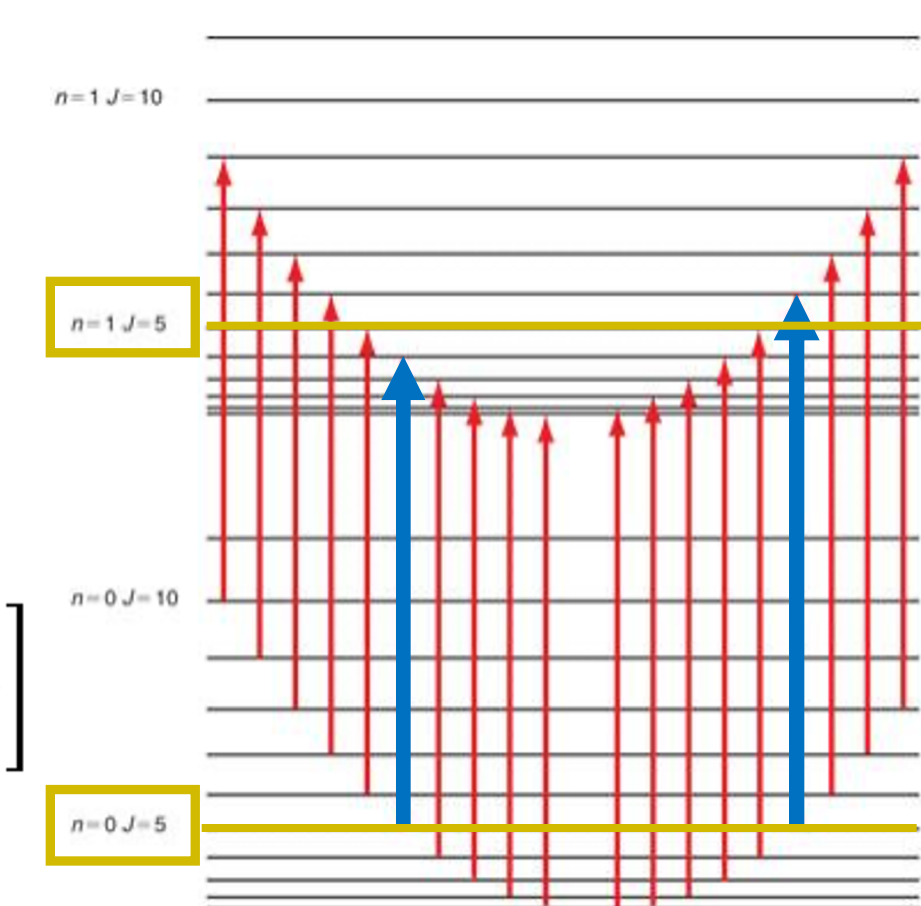
Department of Chemistry & Biochemistry, DePauw University, Greencastle, IN 46135



## Rigid Rotor Model with Morse Oscillator Model

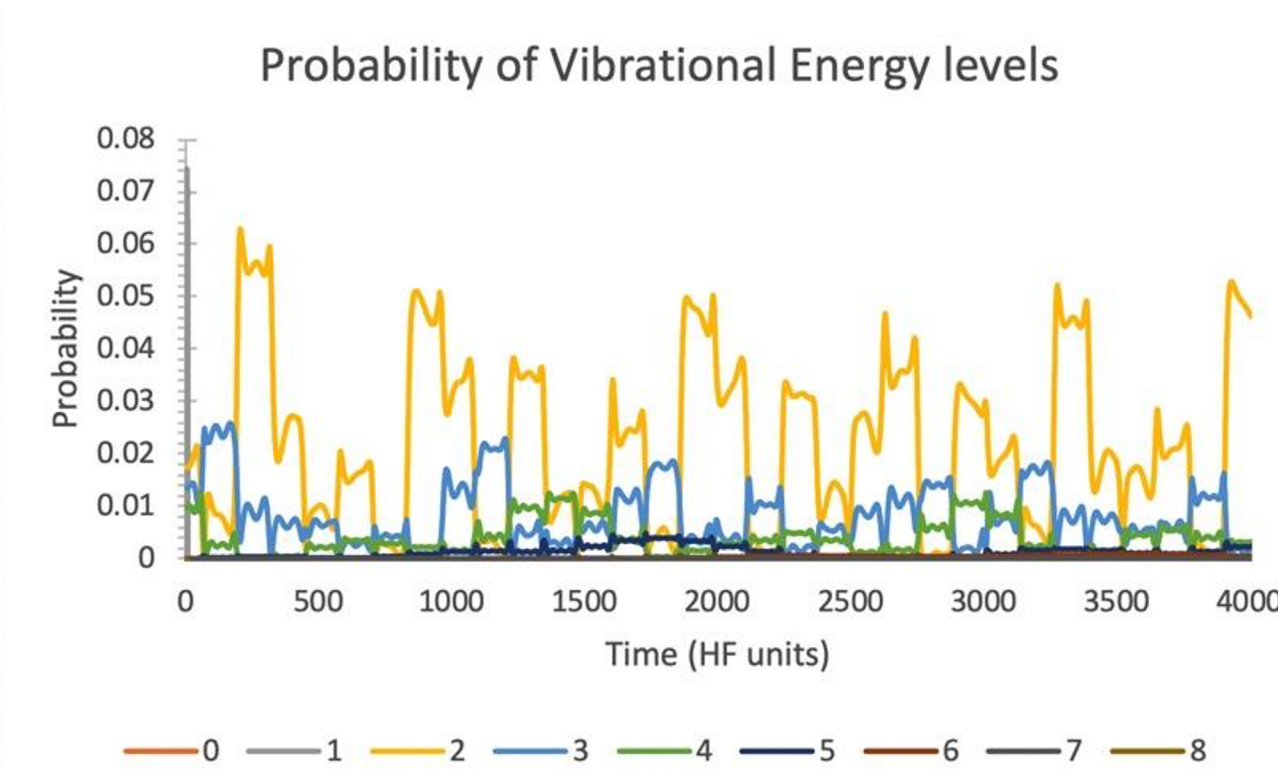
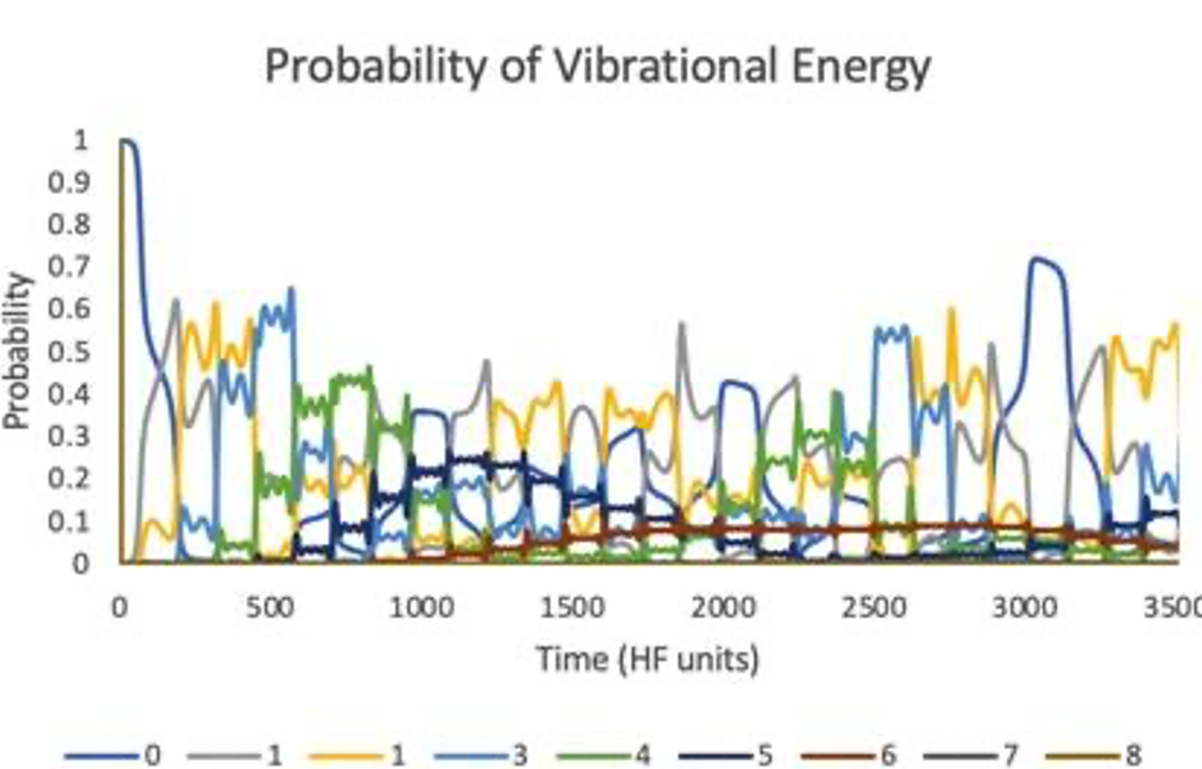
Using the Rigid Rotor model takes into account the vibrational energy levels from the Morse Oscillator Model as well as the rotational energy. Taking into consideration allows our model to be more realistic and increase in subtleties of the energy levels.

Also, this model requires a selection rule ( $\Delta n = +1, \Delta J = \pm 1$ ) due to the mathematics used in the model.



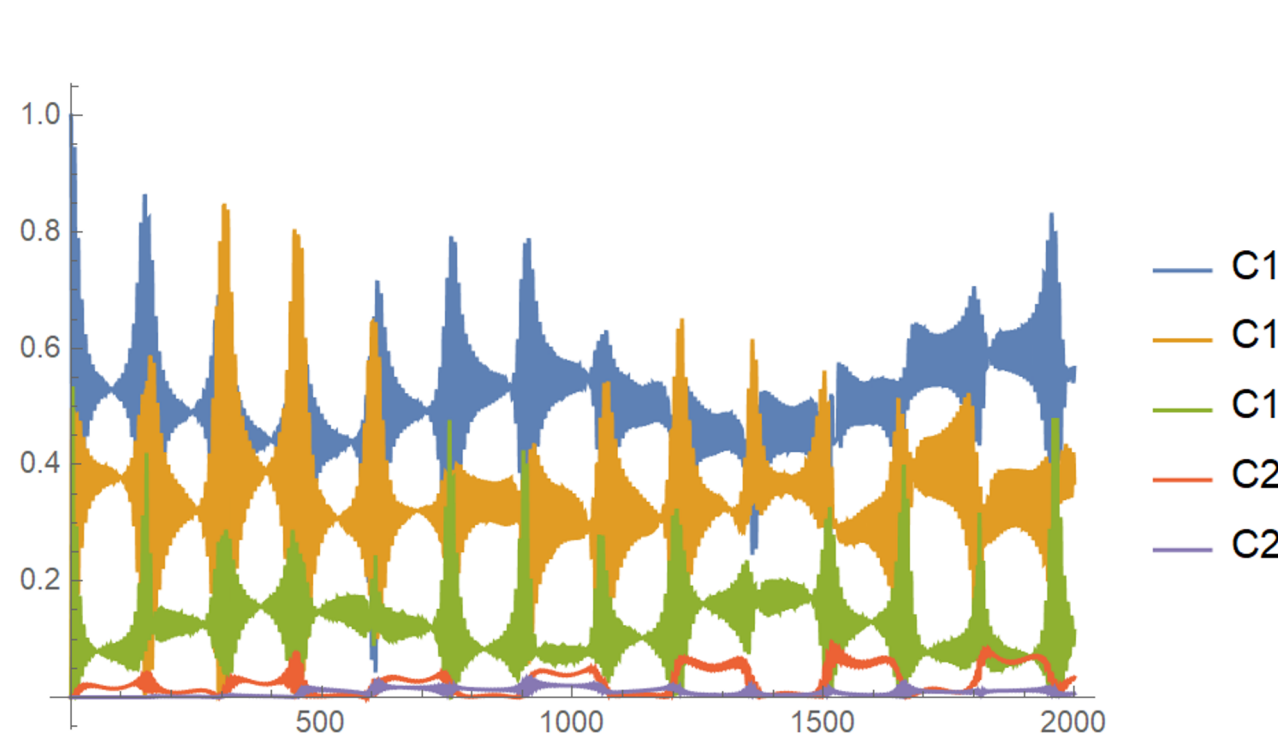
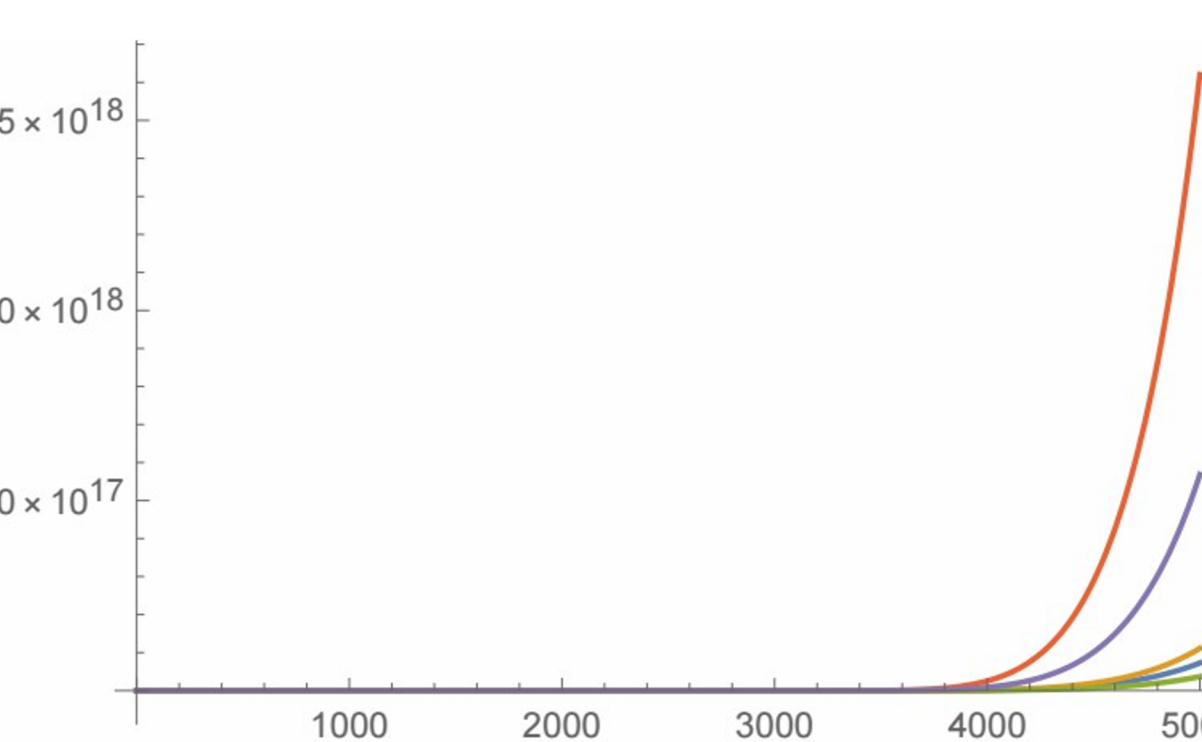
$$E_{n,J} = \left[ \hbar(n+1/2)\omega_0 - \frac{\hbar^2(n+1/2)^2\omega_0^2}{4D} \right] + \left[ \frac{\hbar^2}{2I}J(J+1) \right]$$

## Results



**Figure 1**  
This graph shows the probability of vibrational energy states when five rotational energy states in each vibrational state are also considered in the program.

**Figure 2**  
This figure shows a program with the five rotational states considered as well as starting probability in different rotational states. In the same ground vibrational state.



**Figure 3**  
This graph shows the probability of rotational energy states simulated in Mathematica. Y-axis represents the probability of the energy states. t=(0,5000)

**Figure 4**  
This graph shows the probability of rotational energy states simulated in Mathematica. Y-axis represents the probability of the energy states. t=(0,2000)

## Conclusions and Further Work

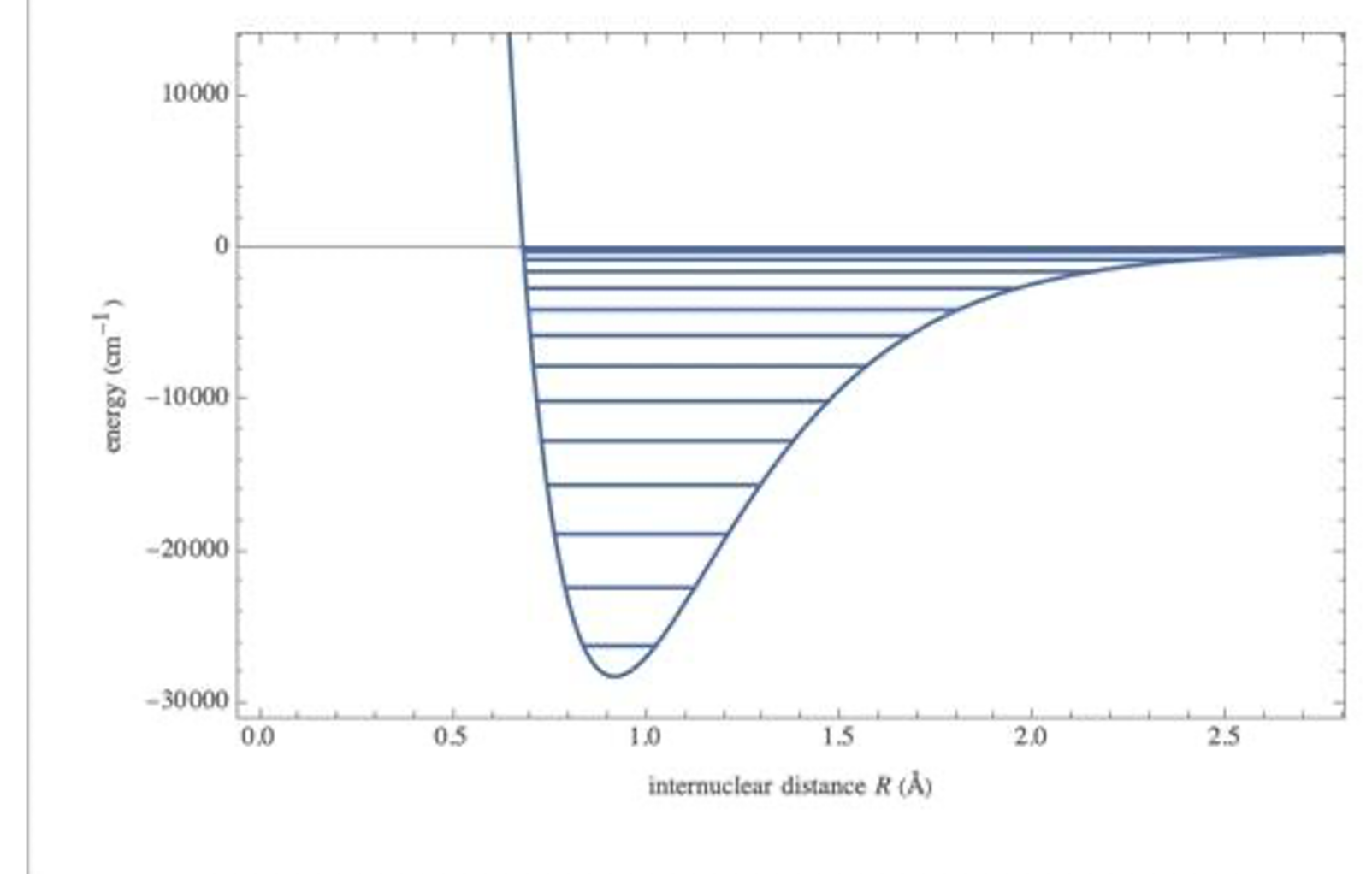
Figure 1 shows that when using the rigid rotor model along with the Morse oscillator model, the probability of vibrational levels changes. This coding only takes into account only a five rotational levels, and more work needs to be done with the program to include more rotational states. Figure 2 uses Boltzmann equation to show that changing the starting probability of the program from  $n=0, J=1$  to higher rotational levels, changes the probability throughout time. This program needs to include more rotational levels to increase the starting probability to equal one. More work that can be conducted with the rigid rotor model, is investigating how these two different energies, vibrational and rotational, interact with each other, and how using different pulse parameters along with the rigid rotor model affect the probability of vibrational states.

## Abstract

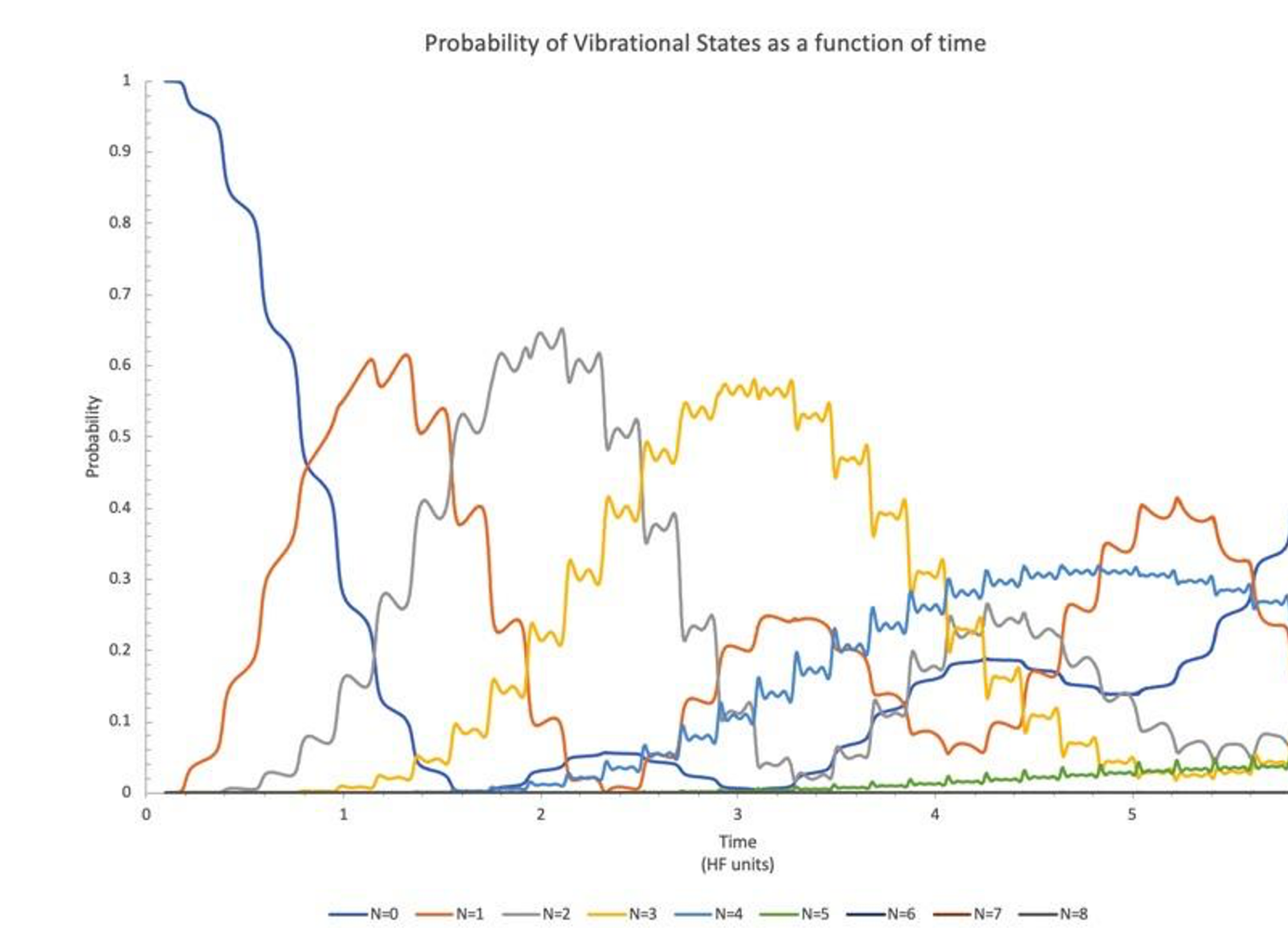
Our goals this summer were to build on previous work in our group modeling ultra-high vibrational and rotational excitation in small molecules via unique pulse sequencing of an infrared (IR) laser. The system was modeled both using Fortran and Mathematica as programming languages. We were able to demonstrate that different numerical techniques for propagating coupled differential equations forward in time led to equivalent levels of vibrational excitation and allowed for identical visualization of molecular state probabilities as a function of time. Work including the rotational motion progressed to the point of being able to see both significant excitation when rotations are included as well as leaking into neighboring rotational states as expected. Much work remains to be done before a full analysis of the rotational excitation can be completed.

## Introduction

Mode selective chemistry allows scientists to isolate a particular mode of a molecule and causes this mode to undergo a change while leaving the rest of the molecule unchanged. Modes can be a bond, functional group, or in our case, a molecular motion like vibration. To be in resonance with the vibrational energy transitions, a picosecond infrared (IR) pulse is used as the energy source. The electromagnetic field of the pulse train is in IR region, and it is pulsed on the picosecond time scale to compensate for molecular anharmonicities and intramolecular vibrational energy relaxation (IVR). We used past work and coding by Professor Gourley to explore new possibilities of the model.



Vibrational energy levels using Morse Oscillator model



Simulation of first 10 vibrational states using Lorentzian pulse train

## Acknowledgements

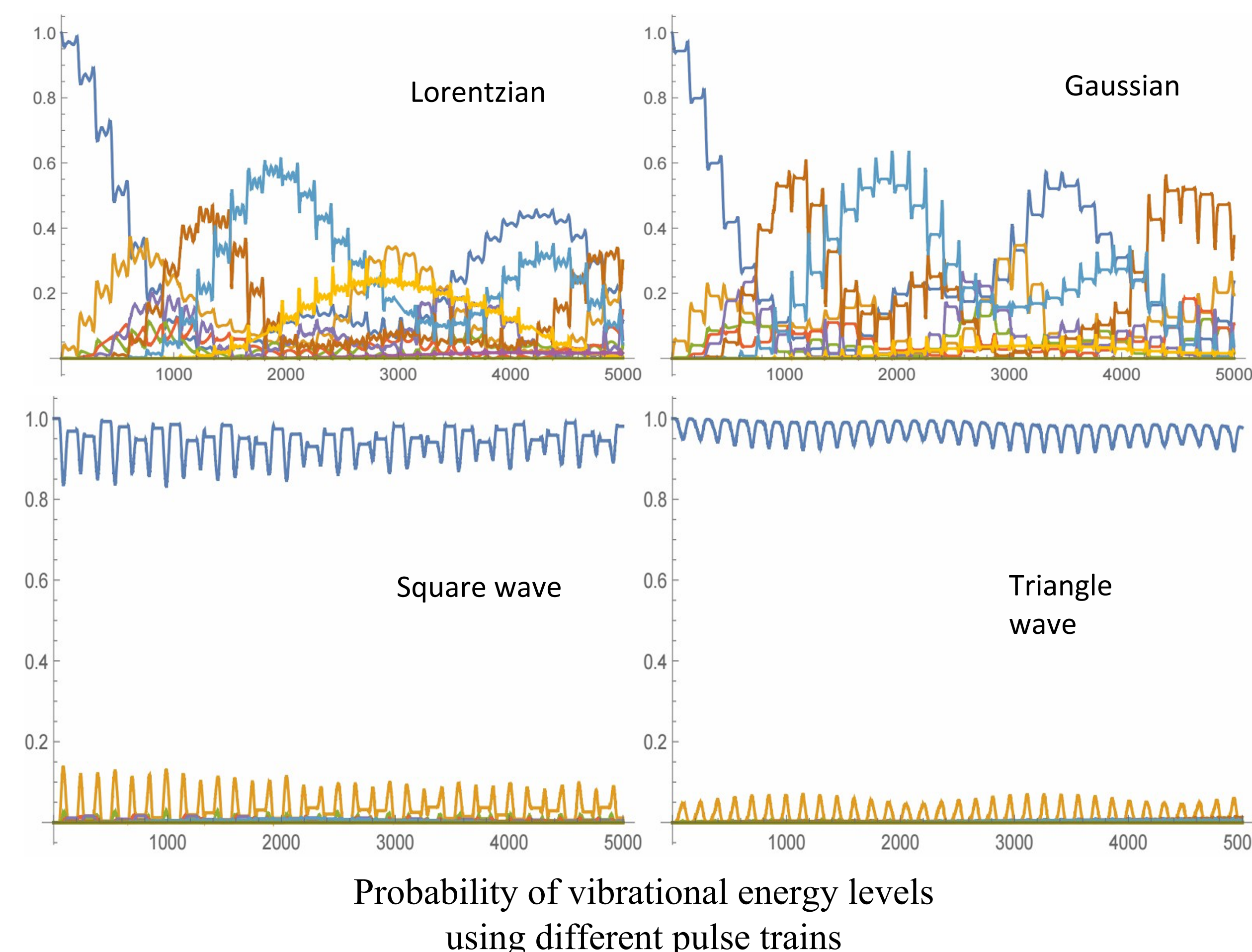
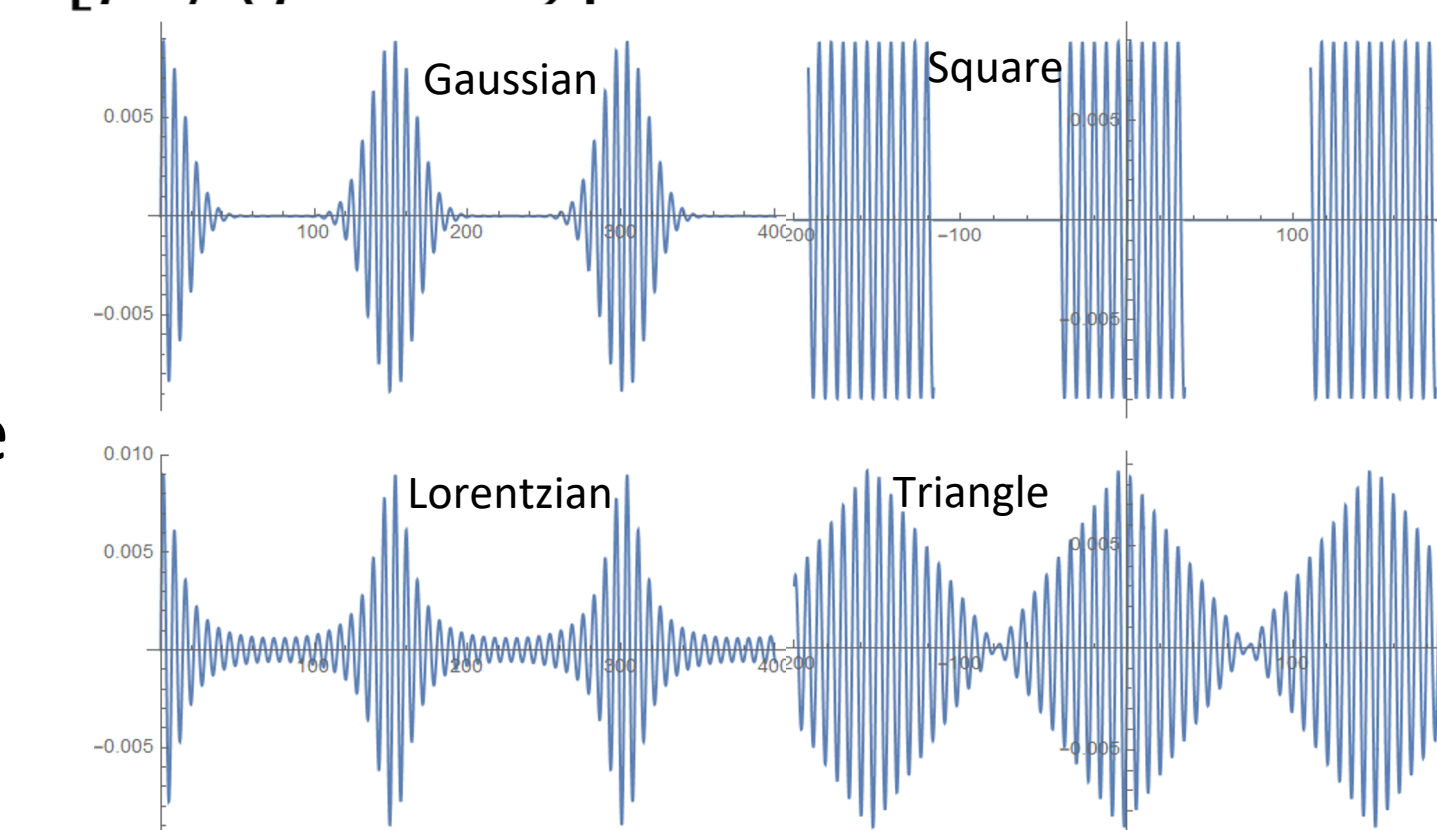
The authors would like to thank Professor Gourley for allowing us to work on this project with her and for providing her expertise on this research. We would also like to thank the Science Research Fellowship program and Chemistry/Biochemistry department at DePauw University.

## Choices of pulse trains

Choices of picosecond pulse trains are important. Professor Gourley chose Lorentzian and Gaussian pulse train in the simulation. SquareWave and TriangleWave are applied in the simulation in addition to the previous pulse shapes.

Lorentzian:  $p(t) = [\gamma^2 / (\gamma^2 + t^2)]$  Gaussian:  $n(t) = \exp(-a^2 t^2)$

Lorentzian and Gaussian shapes works whereas Square and Triangle shapes don't



## Conclusions and Further Work

We've generated results similar to professor Gourley's previous research using both Fortran and Mathematica. Toria used Fortran to generate interesting result for rotational-vibrational model. However, the same model didn't generate good results on Mathematica, which might due to the accumulation of error in the simulation. Square and triangle pulse trains used in vibrational model in Mathematica didn't generate expected shifting of vibrational energy states. Further researches can be done in following ways: 1. Apply well-understood vibrational model to other molecules such as HCl and HCN to test the reliability of the model. 2. Do more test on the rotational-vibrational model to understand its mechanism and refine the model. 3. Test more pulse trains and understand the relationship between the shape of the pulse train and its efficiency of stimulating the energy states.