**SPU Internal Grant Interim[[1]](#footnote-1) or Final Grant Report[[2]](#footnote-2)**

**Academic Year & Type of Grant (FRG, SERVE or Innovation)**

**2015-16 FRG**

**PI Name (and Co-PI’s):**

**Daniel Schofield**

**Original Title of the Proposal:**

**Why is bipyridine planar? Spectroscopic studies of non-covalent interactions in bipyridine**

The Final Project Report must briefly address the following in 1-2 pages:

1. Summarize the project goals and the activities that took place to meet those goals during the grant period. Note who was involved and if anyone was an SPU student.

The goal of the project was to carry out a theoretical analysis of the vibrational spectra of three molecules: biphenyl, 2,2’-bipyridine and 4,4’-bipyrine. Specifically, we investigated how the CH-stretching vibrations in these molecules were affected by the torsional angle between the two aromatic rings. Through an analysis of the calculated spectra we hoped to discover the extent of the interaction between the hydrogen in the ortho-position of one aromatic ring with the atoms of the adjacent aromatic ring. The research team included the PI and two SPU undergraduate students (Joseph Heindel and Elizabeth Knodel). Further details on the specific activities carried out in the grant period were provided in a progress report in August of 2015.

1. What were the major findings? If there are no findings or completed work at this time, what did you learn from carrying out this project that could be applicable to future scholarly works?

The simulated spectra for biphenyl and 4,4’-bipyridine showed a small degree of coupling between the CH-stretching and ring torsional modes. The limited coupling is most likely due to minimal steric interaction between the hydrogen atoms of adjacent rings. We extended the project beyond the molecules described in the original proposal, and were unable to find an example where strong coupling between CH-stretch and vibrational torsion was observed.

1. How were or will the results be disseminated (publication, presentation, creative work, etc. – be as specific as possible)? Please add an addendum or link to completed projects or provide a time-line for future dissemination.

The results of this project have already been disseminated at the Murdock college science research conference in Vancouver, WA. Elizabeth Knodel (one of the student researchers) presented a poster at this conference detailing the results of our study.

1. What future scholarly works will be related to this project?

At this time no future scholarly works will be directly related to this project. However, the skills acquired by the undergraduate students who carried out this project have enabled a great deal of new work that should lead to scholarly products.

1. Is there external funding that you would like to pursue with the [Office of Sponsored Programs](http://blog.spu.edu/csfd/external-grantssponsored-programs/)?

Following the completion of our FRG project we submitted a grant to the Murdock College Research Program for Natural Sciences. This grant application was successful, and we received $45,000 to study how non-covalent interactions affect vibrational spectra in the condensed phase. Although this project is not directly related to the FRG funded project described here, the FRG was extremely helpful in providing perspective for this project.

1. Did you run into any problems or difficulties in completing the project? How were these resolved?

We did not run into any problems or difficulties outside of the usual trials and tribulations of original scientific research.

1. If you had student participation – how did participation in this project further their professional goals or vocational understanding?

This project was invaluable for both of the student researchers who participated in the project. Both students have continued to carry out research under my direction throughout the school year, and Elizabeth is spending the summer of 2016 doing research under my direction. The skills she acquired while funded through CSFD have allowed her to work on a variety of projects in different subfields of chemistry ranging from physical chemistry to biochemistry. Joseph was able to use his research experience to obtain an National Science Foundation funded fellowship for the summer and is working at Sandia National Laboratories in Livermore, CA. Joseph will enter graduate school in chemistry following his senior year, and this project and his subsequent experience have assisted him in vocational understanding.

1. Faculty with a multiple year grant or asking for an extension or reallocation of their grant monies must complete as much of this form as possible as an interim grant report before multiple year disbursement, extension or reallocation can occur. [↑](#footnote-ref-1)
2. When electronically submitting your report to CSFD, please cc: your chair and/or dean (whomever received your original grant notification). [↑](#footnote-ref-2)