Appalachian Colleges Association

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In the summer I had 4 undergraduate research assistants helping study metaphosphate glass compounds. The $1,500 ACA research grant was used to pay for travel and chemicals for this project. My salary ($6,000) and the salary for two students ($2,000 + $2,000 work-study match) came from my Research Corporation grant. The other two students were paid via the Berea College matching portion of this ACA grant. Additional chemical and travel costs were covered using both the Research Corporation and Dreyfus Foundation grants I currently have. Over the last year, I published one paper on the comparison of dynamic-angle spinning and multiple-quantum magic-angle spinning NMR experiments in Solid State Nuclear Magnetic Resonance. Work for this paper was conducted at Stanford and University of California Berkeley (the summer of 1995) while most of the writing and data analysis at Berea (over 1996 and 1997).

During the summer of 1997, a number of major research objectives were achieved. Previously, at OSU the short-term of 1996 and during the summer of 1996, my students were able to conduct switched-angle spinning (SAS) experiments similar to those initiated the summer of 1995. We continued to analyze these spectra of phosphate glasses including a more thorough analysis of the first sample of 59.3% Na_2O and a second sample of 63.7% Na_2O using programs developed last summer by Khaled Sarker. The major outcome of this analysis was to discover that the observed distribution of shifts is essentially the same distribution in both glasses. The easiest model to imagine for these glasses is a pile of phosphate chains of length 2, 3, 4, etc. If you randomly mix these chains together, the net result appears that the NMR spectrum has regions dominated by the chains of length 2, regions dominated by chains of length 3 and so on. So in the two glasses (which have different average chain lengths of 4.49 and 2.64 for the 59.3 and 63.7% Na_2O glasses respectively) the observed spectrum is merely the summation of each of the types of environments and thus changing the Na_2O composition simply shifts the spectrum to increase populations of different chain lengths. This is a new model which has recently been proposed by other researchers and we are currently preparing a paper which details our analysis and will describe how our data supports this model. Previous models have ascribed the shift of the NMR spectrum to overall changes in the population of *d*-orbits on the phosphorus atoms, but this model seems to be inconsistent with the data we have collected.

We continued quantitative analysis of the composition of our samples. The atomic absorption methodology was further explored and refined, though the error limits still remain larger than we would like. This is a continuation of work began last summer by Addis Alemayehu, continued by Alicia Lane and Steve Roberts during the spring term and then Addis again this summer. We are beginning to wonder if we will be able to achieve good enough precision with this method to make the determinations we desire. This fall we are embarking on using the UV/Vis spectrometer to do a similar analysis with hopes that it may produce lower error limits. Secondly, Denis Aliker also continued efforts to improve the gravimetric analysis he developed last summer. As with the atomic absorption project, we are limited by poor precision (approximately 4% in this case) and we would really like to reduce the errors below ±0.5%. Again, this method seems to have reached the limit of its precision and accuracy and we have started looking at an alternative method which precipitates out $MgNH_4PO_4$ instead of the phosphomolybdate, $(NH_4)_3PO_4 \bullet 12MoO_3$, compound. Initial results look promising and we hope to achieve error limits under 1% using this gravimetric method.

Students began large scale computations using *ab initio* calculations on a desktop workstation. We set up GAUSSIAN94 software to run on Dr. Michael Crescimanno's new DEC-Alpha workstation in the physics department at Berea. Myron Vance and Pornippa Vichchulada both became highly skilled in operation of UNIX operating system and using the GAUSSIAN94 program. They did number chemical shift calculations on various adamantanone and phosphate based molecules. The results are highly promising to provide good empirical data to compare to our NMR data coming from the OSU experiments.

The collaborations at OSU and Stanford have been continued at least until we acquire a high-field NMR spectrometer at Berea. At the end of the summer I began to work on a major proposal to the NSF-ILI program to purchase a high field NMR spectrometer at Berea. If this $200,000 proposal succeeds we should have facilities at Berea to do all of my research locally and in addition to help research efforts at other ACA schools if there is interest. Long term goals remain to study additional sodium and potassium phosphate glasses and evaluate the role the cations play in producing order in the Q^2 and Q^1 sites. This ultimately will be evaluated relative to the issue of ionic conductivity.

The overall institutional benefits from this project are reflected in student learning, faculty development and publication of results. The students engaged in this research project have learned a number of new techniques along with understanding a little better the process we call research. They can carry this information with them as they enter graduate school and in particular students who have worked on this project over the last four years have gone on to places such as Johns Hop-

kins biochemistry department and University of Kentucky medical school. Of course the research experience is not entirely responsible for these outcomes, but it certainly has provided one of the bricks which has helped pave the road to success for these students. As far as faculty development, I have shown results from this research at a conference this past spring and will probably show additional results in the future. It also has been the foundation for advancing my knowledge in the fields of analytical and physical chemistry. The institutional benefit stems from the long term continuation of a strong undergraduate research program. Support from organizations such as the ACA and others is what keeps this program active and interesting. In conclusion, I would just like to sincerely thank you at the Appalachian Colleges Association (as well as the Dreyfus Foundation and the Research Corporation) for supporting my research from the earliest stages.