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In the summer I had 3 undergraduate research assistants (Charles Kaiza, Nicholas Ndiege and Tom Bentley) helping study metaphosphate glass compounds. The $4,500 ACA research grant was used to pay for my salary ($3,000, $450 of which has not been given to Berea yet), supplies and chemicals for this project. The salary for three students was paid for by Berea College and the chemistry department. Additional chemical and supplies were covered using both the Research Corporation and Petroleum Research Foundation grants I currently have. Over the last year, I submitted one paper on the chemical shift tensor distribution in phosphate glasses. This paper is currently being revised and I hope to get it published by the end of the year.

During the summer of 1998, a number of major research objectives were achieved. First Charles Kaiza and I developed NMR simulation programs which account for the spinning rate and angle of the sample as well as for a distribution of chemical shift tensors. No other research group has tried to simulate glass spectra at this level, with most researchers assuming Gaussian broadened lineshapes to account for any distributions in the glass. Not only do we simulate slices which are of a single isotropic shift, but we add the constraint of measured dipolar linewidth and distributions of CSA tensors to the program. This means the number of free variables is substantially reduced and the fits are quite reliable. These fits will be added to the paper which I am resubmitting to Journal of Physical Chemistry and will greatly strengthen the value of the results.

We continued quantitative analysis of the chain length distributions of our samples. Tom Bentley got our new high performance liquid chromatograph (HPLC) running and we have been successful at separating out the various phosphate chains using a Hamilton X100-PRP ion exchange column with post-column $Fe(ClO_4)_2$ addition to facilitate detection. Our preliminary results indicate that the glasses are highly stable when dissolved at medium pH and do not decompose into orthophosphate units. We have begun to correlate the distributions observed with the composition and hope that we can improve our models of glass structure using the HPLC results.

Finally, Nicholas Ndiege began large scale computations using *ab initio* calculations on a desktop workstation (DEC-Alpha clone). Nicholas both became highly skilled in operation of UNIX operating system and using the GAUSSIAN94 program. He followed up on earlier work by Myron Vance in calculating di-phosphate chemical shift tensors and began to study the substantially

harder tri-phosphate cluster. Nicholas has demonstrated that the lowest energy bend/stretch available to each cluster is the P-O-P bond angle. This may be easily bent from 130 to 180° and the geometry of this angle in the clusters directly affects the overall size and shape of each cluster (tri- and di-phosphate). The NMR correlations are being used at this point to try to interpret the observed CSA distributions simulated by Charles Kaiza. The combination of the experimental and computational data is giving us new insights into how the chains stack in a phosphate glass.

We received news this summer that we were funded by the NSF-ILI program to purchase a high field NMR spectrometer at Berea. This $200,000 proposal will provide us an instrument at Berea to do NMR experiments I have previously been traveling to OSU and IU to perform. The collaborative work at UK and Centre never quite panned out as hoped, due to difficulty in scheduling and concerns about the difficulty of instrument reconfiguration by the users at those schools. With the new 300 MHz instrument at Berea, we will be able to do all the experiments on campus and will even be able to help other ACA schools who have an interest in pursuing NMR experiments at Berea.. 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. 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. 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.