



**CALIFORNIA STATE SCIENCE FAIR
2004 PROJECT SUMMARY**

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| Name(s) Phillip T. Deutsch | Project Number S0505 |
| Project Title A New "Spin" on the Haasnoot-Altona Equation: Determination of Theta by Variable Solvent and Variable Temperature NMR | |
| Abstract Objectives/Goals The objective of my project is to develop a method of determining the rotational conformational equilibrium about the central C-C bonds of substituted ethanes. Such methods already exist; the goal of this project is to develop a new method, which, unlike existing methods, does not require assumptions regarding the value of the dihedral angle theta for each rotamer. Methods/Materials Nuclear Magnetic Resonance (NMR) spectroscopy provided the raw data from which the conformational equilibrium was extracted. The difficulty lies in interpreting the NMR spectra, which do not clearly display conformational information because of averaging due to rapid rotation around the central C-C bond. To overcome this difficulty, a series of NMR spectra was taken while varying a single environmental parameter such as temperature or solvent. Each observable (such as a chemical shift or scalar coupling) in these spectra is the weighted average of the observables belonging to each conformer, and a linear equation exists that describes this averaging. A (nonlinear) system was constructed from these "averaging equations" for each series and interpreted using inferential methods on the root mean square error statistic. From these systems the conformational information was derived and an estimate of the dihedral angle theta for all conformers was obtained. Results Of the several series used, only one, (1,1 dichloro-2,2 difluoroethane) produced valid conformational information under rigorous statistical scrutiny. All other methods admitted multiple plausible solutions. The information provided by the new method indicated dihedral angles not significantly different from prevailing assumptions. Conclusions/Discussion The primary reason that the variable temperature-coupling constant method succeeded while the others failed was because it provided the greatest number of additional constraints (primarily thermodynamic) that could be used to eliminate plausible solutions. There is no reason that the analysis used for 1,1 dichloro-2,2 difluoroethane could not be extended to any asymmetric substituted ethane. Unfortunately, this new procedure is much more experimentally intensive than the currently prevailing one, but nevertheless allows an analysis independent of assumptions for theta, and it or similar methods should be used in all contexts where such assumptions cannot be safely made. | |
| Summary Statement This project develops new methods of determining the rotational equilibrium of simple ethanes. | |
| Help Received Work was done at the Gates and Crellin Laboratories of Chemistry at Caltech under the supervision of Dr. John Roberts | |