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FINAL TECHNICAL REPORT
DURIP AWARD F49620-95-1-0112
Mark S. Gordon, Department of Chemistry
Iowa State University

The funds awarded were used to purchase two nodes for an IBM SP2 parallel computer ($75,570) and a DEC ALPHA 250 graphics workstation. The AFOSR funds were augmented by funds from other sources to purchase a Power Macintosh for the purpose of graphics development.

These computers are being used for a variety of AFOSR-related research projects.

1. We have developed a graphics interface for our electronic structure program GAMESS. This graphics interface is called MacMolPlt. Its primary function is as a "back-end" interface, meaning that it is used primarily to interpret the results obtained by the quantum chemistry calculations using GAMESS. For example, we can make animations of computed vibrational frequencies, we can animate reaction paths that take a reacting system from reactants through transition state to products, and (using a new feature in GAMESS) we are able animate classical trajectory simulations. The most recent addition to this program is the ability to visualize orbitals. Very recently, we have developed a graphical front end for GAMESS, whoch provides the ability to construct input using a menu. These graphical capabilities greatly enhance our ability to interface with and understand the results obtained using our local SP2 and the much larger SP2 at the Maui Supercomputer Center.

2. We are using the SP2 and the DEC computer to address several important Air Force problems. In the HEDM program, we are studying the potential energy surface for high energy forms of the NO dimer, we have completed a study of high energy structures of fluorine azide, and we are studying several metal-doped hydrogen systems. We have also initiated an investigation of octa-sila cubane. This compound, which has been synthesized using bulky substitiuents, is predicted to be a very promising additive. In the area of silicon chemistry, we are investigating the role of divalent Ti as a catalyst in the hydrosilation reaction, an important industrial process to make new SiC bonds as silicon carbide precursors. We have completed a study of a series of titanatranes, precursors for titanium silicides and carbides, and we have just initiated an investifation of silsesquioxanes.