Get the Most Accurate Geometry Optimization

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This project focused on finding the best combination of basis sets, theories, and engines to run an optimization that is the most accurate with experimental data. The jobs for this experiment were run on the North Carolina High School Computational Chemistry Server and the Shodor Server. The engines used were Guassian and Mopac. The theories used were AM1, PM3 PBE, Hartree-Fock, and B3LYP. The basis sets used were minimal, regular, basic, and accurate. It was found that the different combinations between basis sets, theories, and engines have an influence on how accurate the molecule is when compared to the experimental data. Jobs run using the basic basis set were found to have to most accurate data. Hartree-Fock was the most accurate for lengths, but for angles PBE was the most accurate.