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An Ab-Initio Study of Multiple Conformers of Glycine DANIEL KAPLAN, HANYU ZHANG, Stevens Institute of Technology — The recent combination of new computational chemistry techniques and high performance computational hardware is allowing unprecedented levels of accuracy in the calculations of physical quantities such as potential energy surfaces and rotational-vibrational spectra. In this work, we present calculations of the four most stable conformers of Glycine using the aug-cc-pVDZ basis set and Coupled Cluster Theory. We compare our calculations to experimental values and show that our current calculations differ by less than two percent from measured values, much better than results from previous years. When searching for molecules in the Interstellar Medium this small difference suggests that computational methods are becoming well-suited for the task. The natural question to ask is: at what point will the small deviation from experimental values render our computations just as reliable as experiments? We feel that the current results show that we are indeed close to this goal.

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