Public Abstract
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Title:VARIABLE-TEMPERATURE 1H-NMR AND AB INITIO STUDY OF 5-AMINO-IMIDAZOLE-4-CARBOXAMIDE (AICA): COMPETING PATHS FOR AMIDE-H SCRAMBLING

This thesis explores a previously known molecule 5-amino-imidazole-4-carboxamide (AICA) that matters in the prebiotic synthesis in the interstellar medium. The extensive study on this compound may provide good support for the hypothesis that life begins from outer space. It is very interesting to know this because life formation in planets other than earth could be possible. However, the problem is that existing spectroscopic techniques can not detect such small organic molecules in the infinite universe. This is pretty much like finding a needle in the hay. In addition, gas phase experiment in lab is too expensive, time consuming and dangerous. As a result, two alternative ways have been used: investigating molecules in solutions, and calculating it in computer.

In our research, dynamic NMR techniques and ab initio computation have been carried out to pursue intrinsic structural understanding of molecules. NMR experiment in different solvents gives us the dynamic information and thermodynamic barrier for this process. Then theoretical potential surface analysis provides us with calculated thermochemical data and conformational information of AICA in both gas phase and solution. Isomerization between AICA analogues has been investigated. The calculated data are in line with experimental results. Two plausible mechanisms being responsible for dynamics of AICA in solution are summarized by means of understanding AICA interaction with solvent molecules.

Future work might be done with consideration of less or non polar solvents. This condition is greatly similar to gas phase. The information derived from them will be more helpful to testify the theory.