Quantum Chemistry Meets Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules

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For many years, scientists suspected that the interstellar medium was too hostile for organic species and that only a few simple molecules could be formed under such extreme conditions. However, the detection of approximately 180 molecules in interstellar or circumstellar environments in recent decades has changed this view dramatically. A rich chemistry has emerged, and relatively complex molecules such as C_{60} and C_{70} are formed. Recently, researchers have also detected complex organic and potentially prebiotic molecules, such as amino acids, in meteorites and in other space environments. Those discoveries have further stimulated the debate on the origin of the building blocks of life in the universe.

Spectroscopic techniques play a crucial role in the investigation of planetary atmosphere and the interstellar medium. Increasingly these astrochemical investigations are assisted by quantum-mechanical calculations of structures as well as spectroscopic and thermodynamic properties to guide and support observations, line assignments, and data analysis in these new and chemically complicated situations. However, it has proved challenging to extend accurate quantum-chemical computational approaches to larger systems because of the unfavorable scaling with the number of degrees of freedom (both electronic and nuclear).

In this contribution [1], we show that it is now possible to compute physicochemical properties of building blocks of biomolecules with an accuracy rivaling that of the most sophisticated experimental techniques, and we summarize specific contributions from our groups. We analyze the spectroscopic properties of representative building blocks of DNA bases (uracil and pyrimidine) and of proteins (glycine and glycine dipeptide analogue). Solvation, surface chemistry (dust fraction, adsorption, desorption), and inter- and intramolecular interactions, such as self-organization and self-interaction, are important molecular processes for understanding astrochemistry. Using the specific cases of uracil dimers and glycine adsorbed on silicon grains, we also illustrate approaches in which we treat different regions, interactions, or effects at different levels of sophistication.

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