QUANTUM CHEMISTRY MEETS ROTATIONAL SPECTROSCOPY FOR ASTROCHEMISTRY: INCREASING MOLECULAR COMPLEXITY

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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.

Rotational spectroscopy plays 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.[a] 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, it is demonstrated 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. We analyze the spectroscopic properties of representative building blocks of DNA bases (uracil and thiouracil), of proteins (glycine and glycine dipeptide analogue), and also of PAH (phenalenyl radical and cation).

[a] V. Barone, M. Biczysko, C. Puzzarini 2015, Acc. Chem. Res., 48, 1413