Computational Spectroscopy for Astrochemistry: Increasing Complexity toward Prebiotic Molecules

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Spectroscopy represents the tool of choice for the characterization of molecular systems, in particular the univocal determination of their structures, or in the context of astrochemistry, the identification of molecular species present in interstellar space or other astrochemical environments. The interpretation of most experimental spectra is difficult due to their inherent complexity and computational spectroscopy has shown to be a valuable tool to help unravel the various contributions to the spectrum, allowing for a better understanding of the underlying phenomena.

I will address the challenge of computational support for the identification and characterization of the composition of the interstellar medium and planetary atmospheres or exoplanets soil through spectroscopic signatures. The focus will be on complex organic molecules, including semi-rigid and flexible prebiotic molecules.

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