Quantum Chemical Prediction of Spectra for Key Prebiotic Molecules

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The search for the origins of life necessitates understanding the formation and evolution of complex organic molecules in astrochemical environments [1]. Regions like star-forming cores and protoplanetary disks exhibit rich molecular inventories, and identifying the spectral signatures of key prebiotic molecules is crucial for interpreting astronomical observations [2]. This work presents a detailed quantum chemical investigation of the spectroscopic properties of several astronomically relevant molecules: glycolonitrile (HOCH2CN), aminoacetonitrile (NH2CH2CN), glycolaldehyde (HOCH2CHO), formamide (NH2CHO), methyl formate (HCOOCH3), glycolamide (NH2COCH2OH) and 2-(methylideneamino)acetonitrile (CH2=NCH2CN). These molecules are considered building blocks for more complex biomolecules and have been detected or proposed in interstellar space [3,4].

We employed density functional theory and various functionals to determine conformational spaces, optimize the molecular geometries and estimate vibrational frequencies. Rotational constants were calculated to aid the interpretation of rotational spectra expected from sensitive radio telescopes such as ALMA. Particular attention was paid to identifying key vibrational modes likely to be observed in infrared spectra from space-based observatories such as JWST. Calculated vibrational frequencies were compared with experimental data (where available) and scaled to improve agreement. We investigate the influence of hydrogen bonding, which is particularly relevant in interstellar ice mantles, on the vibrational modes of these molecules using dimer calculations. These findings could aid future observations aimed at unraveling the chemical pathways that lead to the emergence of life's building blocks in the cosmos.

References:

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