# Theoretical Characterization of the Structure and Spectroscopy of $HCNO_2$ Isomers and Applications

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**Abstract**

We carried out a theoretical, fully *ab initio*, investigation of the stable forms of the [H,C,N,O,O] pentatomic molecular system, whose isomers are involved in fundamental combustion and atmospheric processes and are of potential interest for astrophysics. By adopting the MP2 and CCSD(T) electronic structure methods, combined with extrapolations to the complete basis set (CBS) limit, we characterized twenty low-energy isomers, excluding weak van der Waals complexes. For these molecules, we determined a set of geometrical parameters, relative energies, anharmonic vibrational frequencies, IR intensities and fragmentation/formation energies from various atomic and/or molecular fragments. We discuss the relevance of the present findings for the search of new molecular species in astrophysical and atmospheric media and give suggestions for their possible detection in laboratory experiments. The set of data provided by the present work should facilitate the identification of these species from their gas-phase and low-temperature solid matrix spectra, whenever measured.