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Explicitly Correlated Calculations in the CNO System

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Abstract: The CNO role in the atmospheric and combustion chemistry, and its spectroscopic complexity has led to several theoretical and experimental studies in the recent years [1-3]. It is related to some important reactions, involving essential chemical species to several processes such as combustions of nitrogen containing compounds.

It has three linear important species (namely NCO, CNO and CON) in the $^2\Pi$ symmetry, which are Renner-Teller molecules. The NCO is the ground state and is known to be the main product of the $CN + O_2$ reaction [4].

The literature reports several results for the CNO system [5-9], but with the ever-evolving capacity of the computational and experimental techniques these results become inaccurate. For that, we report geometries, frequencies and spin orbit couplings in the state-of-art Explicitly Correlated Multi Reference Configuration Interaction (MRCI-F12). The calculations were carried out in the MOLPRO package, using the MRCI-F12 (including the Davidson correction) and the vqz-F12 basis set. Table 1 lists the preliminary results for the optimized geometries and energies.

Table 1 – Optimized geometries with bond lengths in bohr and energies in ev. Energies are relative to the three isolated atoms.

Species	R_{CN}	R_{NO}	R_{CO}	ε
NCO	2.311	4.536	2.225	−13,629
CNO	2.287	2.297	4.584	−10,921
CON	4.743	2.505	2.238	−8,415

The frequencies and spin-orbit splitting calculations are still being carried. Investigations of the explicitly correlation importance to the properties will be evaluated. Since there is few information in configurations that differ from the linear and there is no potential energy surface (PES) to this system in such high accurate level of theory, we intend to develop two PES (A' and A'' symmetries).

Keywords: Explicitly Correlated, Spin-Orbit Coupling, CNO, MRCI-F12

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