Electron Correlation Effects and Spin Contamination in Electronically Excited States of Interstellar Radicals
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The study of electronic spectroscopy with application to interstellar compounds has recently received increased attention as the need to understand what molecules might be carriers of interstellar spectra increases. Moreover, the astrobiologist's ability to develop a predictive and advancing the field of astrobiology. Interstellar molecules are often of a high energy nature and are found in the so-called DIBs (Dark Interstellar Bands). These bands are observed in spectra taken in the millimeter and infrared regions of the electromagnetic spectrum.

The study of electronic spectroscopy with application to interstellar compounds has been subjected to laboratory study and the resulting spectra compared to interstellar readings. By comparing the laboratory and interstellar spectra, we can identify potential molecular carriers of interstellar spectra. In order to give a quantitative measure as to the accuracy of a given computational method, the Approximate Excitation Level (AEL) is used. This sum of differences between the excited state electron density and ground state electron density provides a diagnostic of the excited states calculated by EOM-CCSD.

The C2H molecule was found to exist in the interstellar medium (ISM) by millimeter wavelength measurements taken in 1974 by the Thaddeus group at the Harvard Center for Astrophysics. It's presence is also important to theories describing the formation of silicate planets. Moreover, its presence has been hypothesized since other silicon containing compounds have been detected there.

A question of interest is the presence of C2H in the interstellar medium. This question has been addressed by computational studies. The C2H molecule was first found to exist in the interstellar medium by millimeter wavelength measurements taken in 1974 by the Thaddeus group at the Harvard Center for Astrophysics. It's presence is also important to theories describing the formation of silicate planets. Moreover, its presence has been hypothesized since other silicon containing compounds have been detected there.

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Mathematical Considerations

In order to give a quantitative measure as to the accuracy of a given computational method, the Approximate Excitation Level (AEL) is used. This sum of differences between the excited state electron density and ground state electron density provides a diagnostic of the excited states calculated by EOM-CCSD.

The AEL is given by:

\[ AEL = \sum_{\text{exc}} \left[ \rho_{\text{exc}}(\vec{r}) - \rho_{\text{ground}}(\vec{r}) \right] \]

where \( \rho_{\text{exc}}(\vec{r}) \) and \( \rho_{\text{ground}}(\vec{r}) \) are the excited state and ground state electron densities, respectively.

In order to determine the AEL, we need to calculate the excited state and ground state electron densities for each excited state. This can be done using various computational methods, such as EOM-CCSD or other more advanced methods.

Systems of Interest

The C2H molecule was found to exist in the interstellar medium (ISM) by millimeter wavelength measurements taken in 1974 by the Thaddeus group at the Harvard Center for Astrophysics. Its presence is also important to theories describing the formation of silicate planets. Moreover, its presence has been hypothesized since other silicon containing compounds have been detected there.

The presence of C2H in the interstellar medium is important for our understanding of the formation of silicate planets.
The ground state of these linear radicals is $^2\Sigma$ for C$_2$H and $^2\Pi$ for SiCH based on our methods.

There is a single strong transition for both of these molecules corresponding to previous work done on these same families of molecules.

Many of the excited states calculated at the EOM-CCSD level of theory give questionable results since they have AEL values substantially greater than 1.0. These questionable states seem to correspond to the states with the largest differences between the UHF and ROHF methods.

CC3 excited states seems to reduce these differences for most of the states in comparison to the EOM-CCSD levels of theory. These differences between the UHF and ROHF methods.

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