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Development of explicitly correlated congruent transformed Hamiltonian MIKE BAYNE, Department of Chemistry, Syracuse University, JOHN DROGO, East Syracuse Minoa High School, ARINDAM CHAKRABORTY, Department of Chemistry, Syracuse University — The central idea of the explicitly correlated congruent transformed Hamiltonian (CTH) method is the treatment of the Coulomb singularity in the Hamiltonian by performing congruent transformation using an explicitly correlated wave function. However, unlike the transcorrelated methods, the CTH is Hermitian and amenable to standard variational methods. The variational solution of the CTH was obtained using FCI and the comparison between the transformed and untransformed calculation will be discussed. We found that the CTH dramatically improves the convergence of the FCI expansion. The CTH can also be represented in the occupation number (ON) space, however this representation is approximate due to the finite size of the underlying basis. Analogous to the diagrammatic summation in MBPT, we have developed partial infinite order summation (PIOS) for improving the CTH calculation in ON space and analysis of the real space, ON and ON-PIOS calculation of CTH will be discussed. The CTH has been applied to a series of 10 electron systems and comparison of the results with other methods will be presented. Preliminary results on the excited state of water will be compared with R12-MP2 and MRCI methods. The size-consistency of the CTH method was numerically analyzed and will be discussed.

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