Accuracy of Excited State Spin-Component-Scaled CC2 potential energy surfaces

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Benchmark calculations with the Spin-Component-Scaled CC2 variants SCS-CC2[1,2] and SOS-CC2[3] are presented for the electronically excited valence and Rydberg states of small and medium-sized molecules. Besides the vertical excitation energies and excited state gradients, the potential energy surfaces are also investigated via scans following the forces that act in the Franck-Condon region. The results are compared to higher level methods CCSD, CCSD(T)(a)* and CCSDT, as well as to the regular CC2. For the latter, serious flaws have been revealed by an earlier study.[4] The results indicate that a large fraction of these flaws disappear if spin-component-scaling is employed, making these variants attractive alternatives of CC2, offering competitive accuracy of vertical excitation energies of both valence and Rydberg type states, reliable potential energy surfaces, while also maintaining a low-power scaling computational cost with the system size.

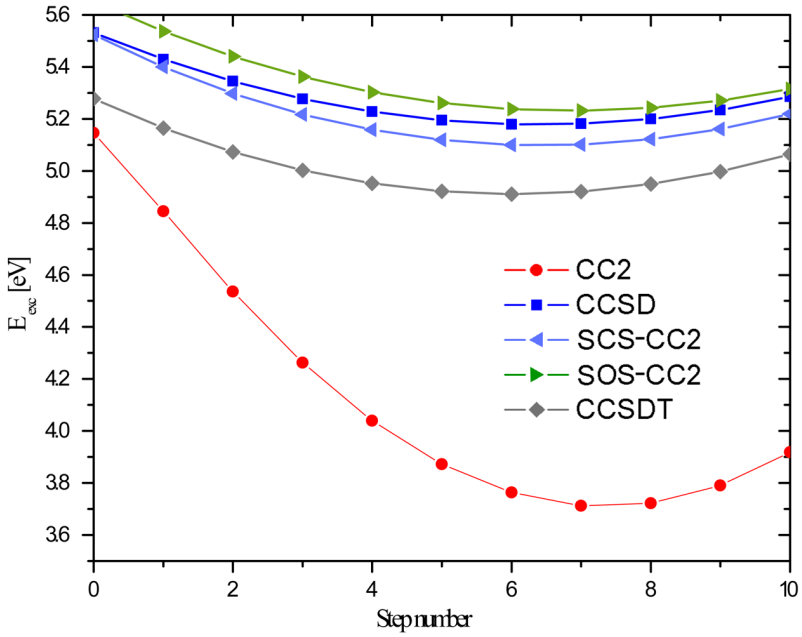

Figure 1: : Illustrative potential energy surface scan for cytosine.

References

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