Quantum Chemistry on Quantum Computers: A Method for Preparation of Multiconfigurational Wave Functions on Quantum Computers without Performing Post-Hartree–Fock Calculations

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Supporting Information

Contents

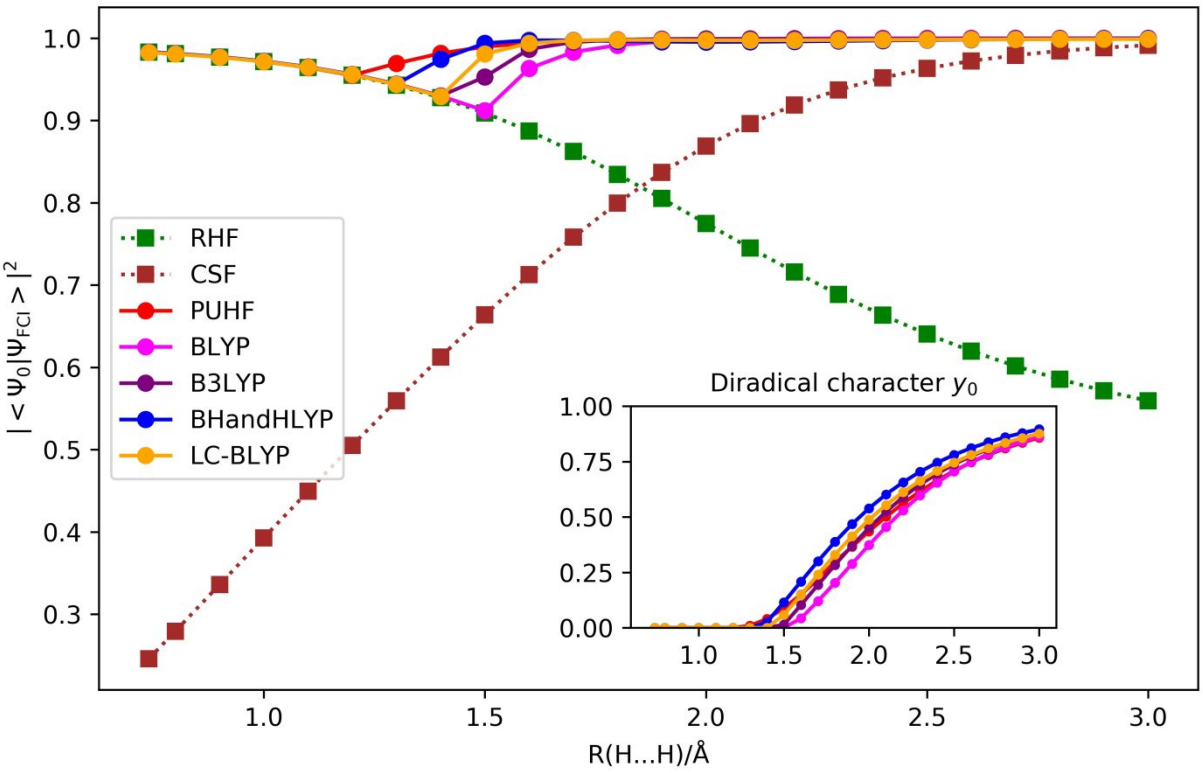

Figure S1: Square overlap between the full-CI/cc-pVDZ wave function of the ground state and two-configurational wave functions using diradical characters computed from DFT in H_2. Inset: Diradical character y_0 calculated from the occupation number of natural orbitals.

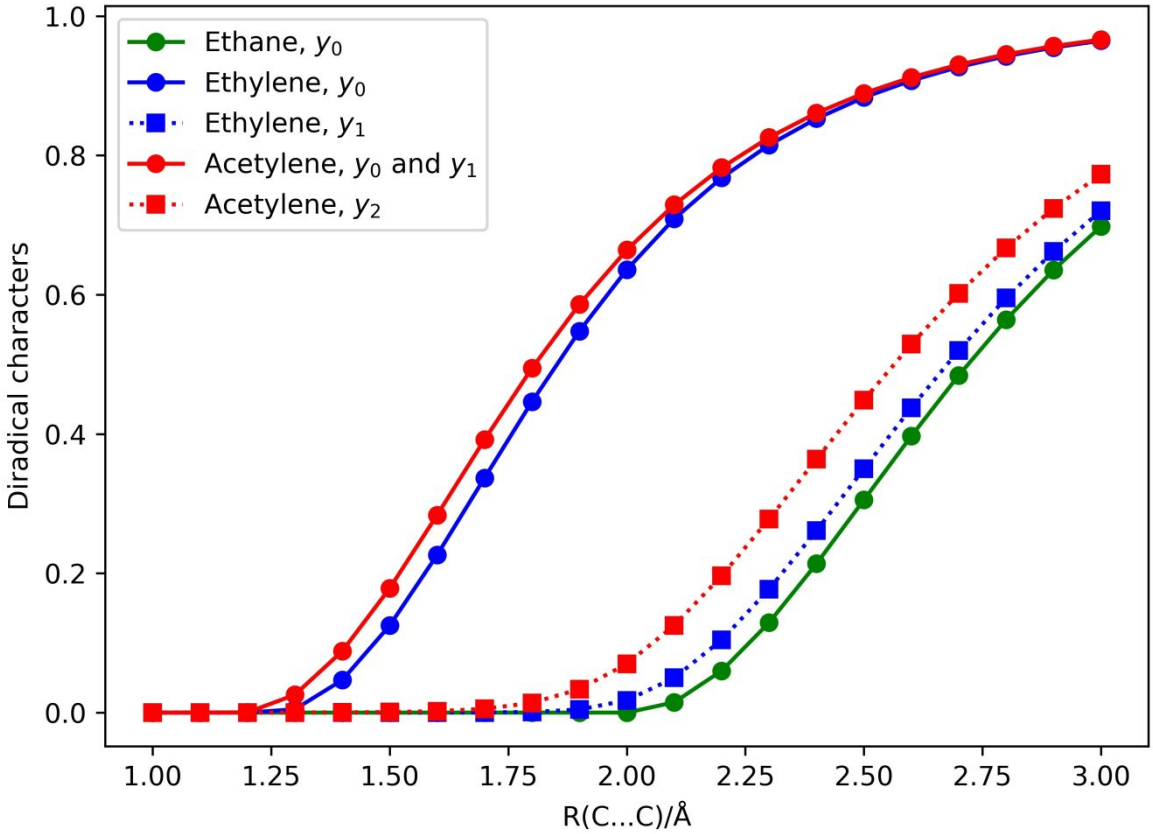

Figure S2: Diradical characters of ethane, ethylene and acetylene calculated from the spin-projected UHF.

Table S1: Square overlap of the initial guess and CAS-CI wave functions in phenylene-1,4-dinitrene.

Initial guess wave function	Square overlap with the CAS-CI wave function	
	Without spin projection	With spin projection
RHF	0.3894	
Use y_0	0.8754	0.8754
Use y_0 and y_1	0.8782	0.9119
Use y_0, y_1, and y_2	0.8827	0.9203
Use y_0, y_1, y_2, and y_3	0.8974	0.9286
Use y_0, y_1, y_2, y_3, and y_4	0.8986	0.9298