QUANTUM MONTE CARLO CALCULATION OF SELECTED PROPERTIES OF PROPARGYL RADICAL AND OTHER HYDROCARBON SYSTEMS.

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We apply the quantum Monte Carlo method with effective core potentials to the propargyl radical, C_3H_3, and its cation and anion. Properties computed and compared with other theoretical and experimental results include heats of formation, electron affinity, and ionization potential. The study of C_3H_3 is important in understanding soot formation in hydrocarbon flames. Other systems that will be discussed are acetylene and ethylene. Binding/atomization energies for the latter systems are found to compare very favorably with experiment.

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