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

JOHN A. W. HARKLESS, WILLIAM A. LESTER, JR., Chemical Sciences Division, Lawrence Berkeley National Laboratory and Department of Chemistry, University of California, Berkeley, CA 94720-1460.

We apply the quantum Monte Carlo method with effective core potentials to the propargyl radical, $\text{C}_3\text{H}_3$, 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 $\text{C}_3\text{H}_3$ 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.

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences Chemical Sciences Division of the U. S. Department of Energy under Contract No. DE-AC03-76SF00098.

JAWH is a Bell Labs Cooperative Research Fellowship Program fellow.