

Abstract Submitted  
for the 4CS19 Meeting of  
The American Physical Society

**A Quantum Mechanical Study of Role of C<sub>60</sub> for Origin of Interstellar Life** JOSE PACHECO, AJIT HIRA, DAVID NUNN, RAMAKRISHNA KHALSA, ARRICK GONZALES, TINO PACHECO, Northern New Mexico College — Understanding the physical and chemical properties of small organic molecules is important for exploring the origin of life. This is a theoretical study of the interactions of a couple of C<sub>60</sub> fullerene molecules with small organic molecules. Our study began with calculations to study the interactions of C<sub>60</sub> with CO and CO<sub>2</sub> molecules, using ab-initio methods based on Density Functional Theory (DFT) and some molecular dynamics (MD). We also performed calculations for the interactions of CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>4</sub>H<sub>10</sub>, C<sub>6</sub>H<sub>6</sub>, CH<sub>3</sub>OH and C<sub>2</sub>H<sub>5</sub>OH molecules with the C<sub>60</sub> fullerene. Some of the important properties of interest in our calculations on these complexes were binding energies, molecular geometries, bond-lengths, ionization potentials, and electron affinities. It should be noted that there have been recent reports on the detection of similar organic molecules in abundant quantities in outer space. We will also present the possible implications of our results for the origin of life in interstellar space and on Earth. Future work will include some experiments to benchmark our computational results..

Ajit Hira  
Northern New Mexico College

Date submitted: 18 Sep 2019

Electronic form version 1.4