Abstract Submitted
for the CAL11 Meeting of
The American Physical Society

FTIR Spectroscopy and Density Functional Theory of the 1474 cm^{-1} Absorption in C$_n$ Carbon Cluster Spectra[1] MEKENA MCGREW, St. Mary's College of California, CHRISTINA LE, W.R.M GRAHAM, Texas Christian University, TEXAS CHRISTIAN UNISVERSITY MOLECULAR PHYSICS LAB TEAM — The identification of the infrared frequencies of carbon clusters is significant for astrophysical and material science research. By using FTIR spectroscopy, density functional theory, and argon matrix trapping numerous C$_n$ carbon clusters have been observed in the Nd:YAG laser ablation products trapped in solid argon. An unidentified absorption at 1474 cm^{-1} has been observed in our experiments, and ^{13}C isotopic shift measurements and DFT calculations have been performed to test potential C$_n$ candidates for the carrier of the band. The number and relative intensities of the isotopic shifts suggest a molecule consisting of 4 or 6 atoms. Simulated ^{13}C shift spectra have been calculated for a variety of 4- and 6-member C$_n$ structureusing the B3LYP functional and ccPVDZ basis set. Potential sources of the 1473 cm^{-1} band will be discussed.

[1]National Science Foundation Grant PHYS-0851558

Mekena McGrew

Date submitted: 29 Sep 2011 Electronic form version 1.4