

Studies of Cyanoacetylene Oligomers: Cyano-Substituted Cyclobutadienes, Dewar-Benzenes, and Benzenes

Jessica L. Menke,^a Robert J. McMahon,^a Henning Hopf,^b and Jens-Uwe Grabow^c

^a Department of Chemistry, University of Wisconsin, Madison, WI 53706

^b Technische Universität Braunschweig, Braunschweig, Germany

^c Gottfried-Wilhelm-Leibniz-Universität, Hannover, Germany

menke@chem.wisc.edu

Cyanocarbons are known to be abundant in the interstellar medium (ISM) and in the atmosphere of Titan. Terrestrially, they are interesting due to their high reactivity with electron-rich molecules. The reaction of cyanoacetylene with [2,2]paracyclophane produced cyano-substituted benzene derivatives as side products – hinting at possible reaction pathways involving dimerization and trimerization. Dicyanocyclobutadienes and tricyano-Dewar-benzenes were computationally studied (B3LYP/6-31G*) as possible intermediates in the proposed reaction scheme (shown below). Dipole moments and rotational constants were also computed to help interpret laboratory microwave rotational spectra. These spectra can, in turn, be used to determine if these species are present in the ISM. Additional computational studies have been completed on other cyano-substituted cyclobutadienes and their isomers.

