LASER SYNTHESIS AND SPECTROSCOPY OF PYRENE DIMERS

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Laser desorption time-of-flight mass spectrometry (LD-ToF-MS) experiments on pressed-pellet samples of polycyclic aromatic hydrocarbons (PAHs) exhibit the formation of covalently-bonded dimers at masses (m/z) of 2M-2 and 2M-4 (where M is the parent mass). Through replication of these LD-ToF-MS conditions at higher throughput, PAH dimers have been produced and collected in milligram quantities. The formation of the covalently-bonded dimers was confirmed under similar LD-ToF-MS conditions and through HPLC separation with a UV-Vis detector. For collected samples of pyrene, differential sublimation has removed the residual monomer to leave a mixture of dimerized pyrene. Decrease of the monomer mass peak was confirmed using LD-ToF-MS, and the samples are analyzed using several spectroscopic methods, including UV-Vis, IR, and Raman spectroscopy. Theoretical studies of possible dimer structures have been calculated using density functional theory with the CAM-B3LYP method at the def2TZV level of theory using the Gaussian 09 program. Theory calculations were calibrated and checked by comparison with the monomer samples, and used to determine the lowest energy dimer structures. The simulated spectra were compared with collected spectra of isolated dimers to determine the contributing structures of the dimerized PAHs.