Determination of Atomization and Combustion Energies of PAHs via Accurate Quantum Mechanical Model Chemistries

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In the last decade the attempt of an original, up-to-date, and more accurate understanding of physical-chemical properties such as stabilities and reactivities of single molecules constituting stable oligomeric structures, has been a paramount challenge in materials science and engineering. The investigation of these classes of structures will provide contributions to day-to-day aspects relevant to such as national homeland security, the environment and welfare, but possibly also to the answering of broader questions such as the origin of Life outside of Earth. The overall objective of this research project is to investigate at the quantum mechanical level intermolecular interactions occurring between molecules forming organic solid materials. This project initially related to the determination of atomization energies; however, it also came to include the heats of combustion of monomers for several PAHs at different temperatures. Both complete and incomplete combustion reactions are being studied, in order to pose quantitative foundations for the investigation of soot formation in the atmosphere. To collect this information, geometry relaxations and frequency calculations were performed on nearly 50 molecules. The results obtained so far allowed to build a trendline which in the future will be used as a base to write a polynomial power series able to extrapolate atomization energies and heats of combustion for molecules containing 20 or more carbons. Approximated calculations were performed at B3LYP-DFT level in combination with 6-311G, aug-cc-pVDZ, and aug-cc-pVTZ basis sets, and were compared to the composite method CBS-QB3 which, for the purposes of this work, is considered to return "true values".