Quantum Mechanical Studies of Five, Seven, and Eight-Membered Enediynes

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Enediyne molecules have tremendous potential in the field of anti-cancer drugs. These molecules can cyclize into benzyne diradicals, which destroy cells by abstracting hydrogens from the DNA, leading to DNA cleavage and cell death. When the enediyne molecules bind with cancer cells, this beautiful mechanism can be utilized against tumor growth. However, the specificity for cancer cells is not yet achieved. In this project, the cyclization energetics of five, seven, and eight-membered molecules with the enediyne moiety are studied using quantum mechanical methods. These results will provide insight into how different structural variations in the enediyne moiety affect the energies of the cyclization pathway and how the aromatic driving force might be harnessed in the design of triggered warhead drugs. Overall, the study contributes to the ultimate goal of finding ways in which the cyclization of enediyne molecules can be controlled and used specifically against cancer cells.