Combustion Reactions of the Constituents of Asphaltene

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As the light sweet crude oil resources deplete all over the world, it is necessary to find other sources of energy. Oil shale is one of those potential sources that is not being used on a large scale because of the higher financial and environmental costs of processing. Conservative estimates of global reserves exceed 2.8 trillion barrels of recoverable oil, which means that oil shale solely can meet the global energy demands for nearly a century. So, the main objective of my project is to develop a theoretical understanding of the energies and mechanism of combustion reactions of the constituents of asphaltene, which is an integral part of oil shale. My project studies the combustion reactions in which diatomic oxygen/nitrogen attacks the asphaltene constituent in-plane from both the sulfur and non-sulfur ends. The constituents studied were thiophene, methylthiophene and benzylmethylthiophene. The reaction species were geometrically optimized using: B3LYP/6-31G*, B3LYP/6-311++G**, and MPWB1K/6-311++G** levels of theory and calculations were performed on both the singlet and triplet surfaces. *Guess=mix,always* was used to break the orbital symmetry in all sets of calculations and vibrational frequency analysis was used to confirm maxima and minima on the potential energy surfaces. It was found that the combustion reaction does not take place when the diatomic oxygen/nitrogen attacks the asphaltene constituents from the non-sulfur side. The energy barriers for the triplet surfaces were lower an in all cases, the barriers for reactions with benzylmethylthiophene being the lowest.