

Pyrolysis and Combustion of Oil Shale Constituents

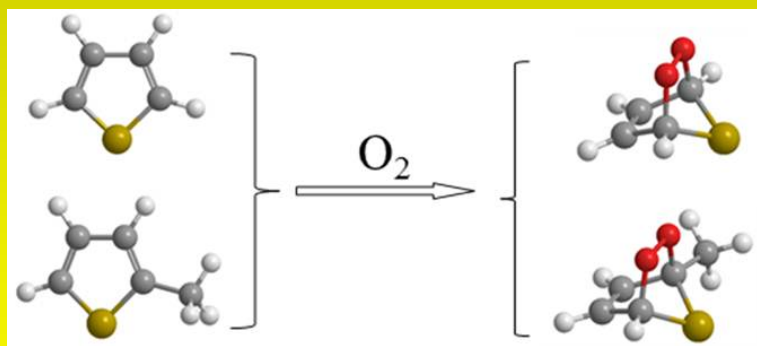
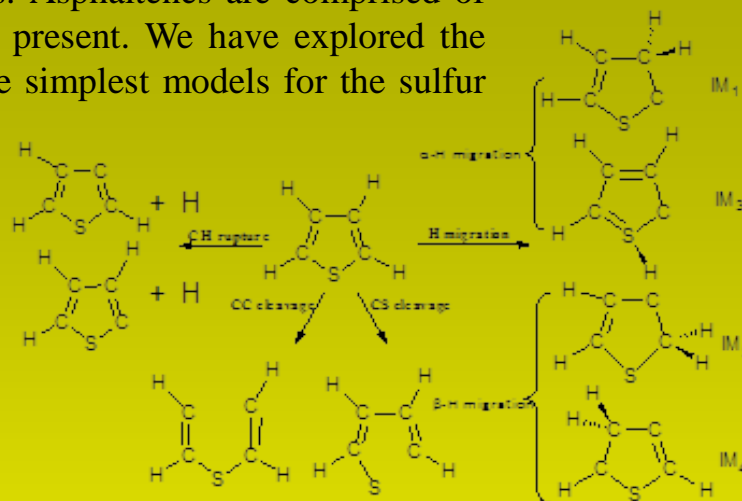


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Oil shale is a form of alternative energy that contains asphaltenes. Asphaltenes are comprised of alkyl-substituted heteroaromatic compounds. Sulfur is known to be present. We have explored the pyrolysis and combustion of substituted thiophenes as these are the simplest models for the sulfur-containing, alkylated heteroaromatic compounds found in oil shale.

Thiophene pyrolysis and combustion processes were investigated using density functional and *ab initio* quantum chemical techniques.

Pyrolysis: The dominant mechanism for pyrolysis is 1,2 H-migration involving two competitive product channels, namely, $C_2H_2 + CH_2CS$ and $CS + CH_3CCH$.



Combustion: The barriers for reaction with triplet oxygen are all significantly large; however, favorable reactions with singlet oxygen proceed via 2+4-cycloadditions leading to endoperoxides.

Radical Recombination: Formation of O_2 , OH and H_2O are important pathways in the radical recombination reactions of 2-thienylmethyl + HO_2 .

