Quantum chemistry calculations of activation energies for oxidative cracking and reutilization of heavy organic materials

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Quantum chemistry calculations were performed in order to estimate the activation energies as well as provide structural and surface data from oxidative cracking processes. Three transition mechanisms of oxidative cracking were investigated, i.e. carboxylic acid–paraffin, alcohol–aldehyde and alcohol–ketone, indicating smaller activation energies for the latter, which is provided by the tertiary carbon present in the chain. The activation energies of oxidative cracking of the model molecule C16 (methyl-pentadecane, relative to the alcohol–ketone mechanism) were smaller (about 2.5 kcal/mol) than polypropylene oxidative decomposition (15.5–17.9 kcal/mol), which would make possible the application of the first mechanism for the reutilization of heavy organic materials.