

## Jersey Ghettos/Garbage Sights

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A quantum chemical study of the OH radical initiated oxidation of tert-butyl alcohol in the presence of water vapor. The rate constants of the OH radical initiated oxidation of tert-butyl alcohol (TBAL) were evaluated at the B3LYP/6-31+G\* level of theory in the presence of water vapor. The temperature dependence of rate constants for each channel was also studied at the same level. The overall reaction rates were reduced in the presence of the excess water vapor, as a result of the hydrogen abstraction from the alcohol by the hydroxyl radical and the intramolecular recombination of the OH radical produced in the abstraction step. The temperature dependence of the rate constant of the process decreased with increasing temperature. The difference in the H-abstraction pathways of TBAL by the OH radical was evaluated by means of a detailed analysis of the energetics and the thermal statistical distribution of the stationary points along the reaction paths. The path chosen by the reaction was not a direct reaction from the OH radical-in

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