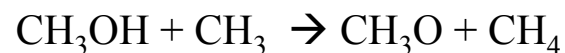
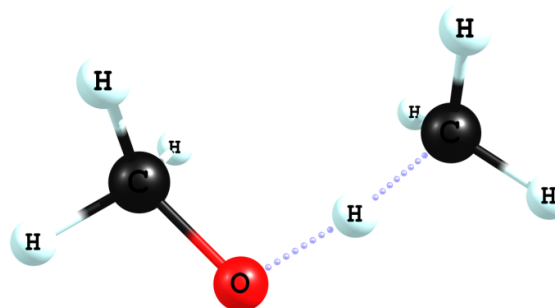
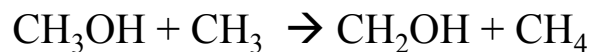
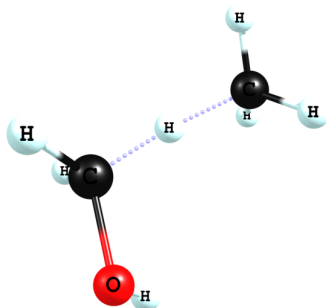
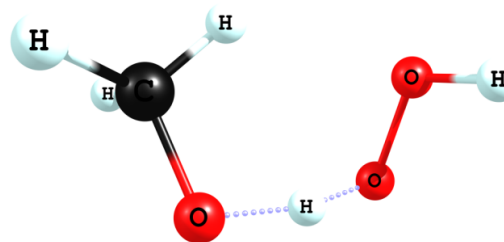
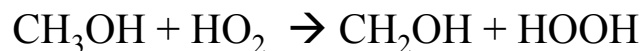
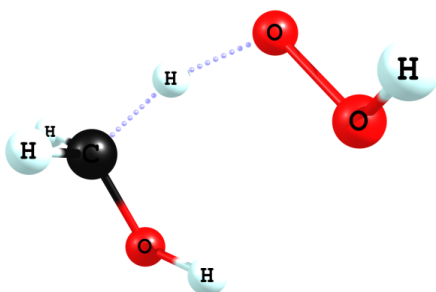


Transition states for reactions of alcohols with the hydroperoxyl and methyl radicals



We tested several high-quality quantum chemical methods for the thermochemistry and barrier heights of the above reaction systems, and we found that the explicitly correlated CCSD(T)-F12b/jul-cc-pVTZ method is very accurate at a cost that is affordable even for larger systems. [I. M. Alecu and D. G. Truhlar, to be published]

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