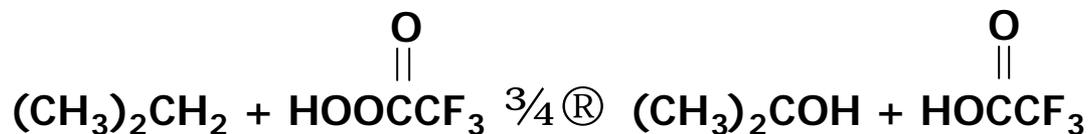


Pilot-14 Highlight

EMSL

The hydroxylation reaction of alkanes by peroxy acids occurs readily even at room temperature (Camaioni et al. J. Org. Chem., **2001**, 66, 789-795).



A non-radical mechanism affords alcohols with high regio- and stereospecificity. High-level ab initio calculations find a biradicaloid-zwitterionic transition state consistent with a concerted pathway and observed reactivity/selectivity.

Transition State (B3LYP/6-311+G**)

