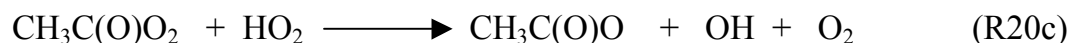


## ABSTRACT

### THEORETICAL STUDIES OF ACETYL PEROXY RADICAL REACTIONS IN THE GAS PHASE

The reaction of peroxy radicals ( $\text{RO}_2$ ) with hydroperoxy radicals ( $\text{HO}_2$ ) represents an important chemical sink for reactive intermediates generated during the formation of air pollution. Recent experimental work<sup>1</sup> has shown that the reaction of acetyl peroxy radicals ( $\text{CH}_3\text{C}(\text{O})\text{O}_2$ ) is more complex than previously thought, and proceeds via three reaction pathways (R8a-c):



with branching ratios of 0.4, 0.2 and 0.4 for 8a, 8b, and 8c, respectively. In this work, a plausible reaction mechanism to explain these reaction yields is proposed. To develop this reaction mechanism, master equation calculations and kinetic simulations were performed using results from quantum calculations on reactant intermediates and transition states. The calculations show that the mechanism is consistent with experimental yields, and suggest that reaction R8c may occur for a number of peroxy radicals generated during smog formation.

Manuel Contreras Arroyo  
August 2005