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The Mechanisms Criegee Intermediates with H_2O Reactions in Atmosphere

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Using quantum chemistry methods CCSD(T)/6-311++G(2d,2p)//WB97XD/6-311++G(d,p), the reaction pathways and mechanisms of CI (i.e. CH_2O_2, CH3CHO_2 and (CH3)2CO_2) with H_2O were investigated. The result indicates that the main products are hydroperoxide for the three reactions, occuring with a pre-reaction complex and the lowest energy barrier to the overall potential energy surfaces. Therefore, the methyl substitution make minor contributions to the three reactions to the dominant products. Moreover, the dominant channel in reactions of H_2O with a series of CI have been studied to develop structure-activity relationships and to understand the characteristics of criegee intermediates (C1-C10)in atmosphere. The current result implies that the stablization energy of pre-complexes and barriers in these reactions are close to each, therefore, the alkyl substitution effect is negligible.