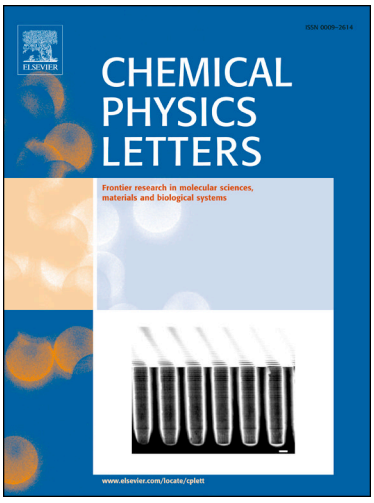

Research paper

Mechanistic and kinetic study on the reaction of methylperoxyl radical with atomic hydrogen

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Mechanistic and kinetic study on the reaction of methylperoxyl radical with atomic hydrogen

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Abstract: Singlet and triplet potential energy surfaces for the CH_3O_2 with H reaction have been investigated computationally to propose the reaction mechanisms and possible products. On the singlet PES, addition-dissociation was located. At 3.65 Torr with He as bath gas, the formation of $CH_2O + H_2O$ channel is dominated at the whole temperature range. Furthermore, the predicted rate constants for $k_{CH_2O+H_2O}$ at 298 K 3.65 Torr of He agree well with the available experimental values. The pathways on the triplet PES will not compete with the pathways on the singlet PES in kinetically.