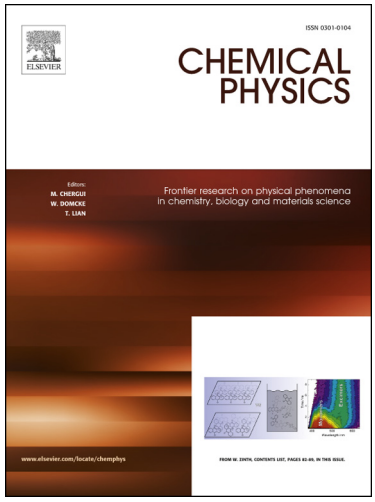

Mechanistic and kinetic study on the reaction of Pyrrole (C_4H_5N) with $O(^3P)$

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Mechanistic and kinetic study on the reaction of Pyrrole (C_4H_5N) with $O(^3P)$

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Abstract: The mechanism and kinetic for the reaction of Pyrrole + $O(^3P)$ has been investigated using CCSD(T)/cc-pVDZ//M06-2X/6-311++G(d,p) method in combine with multichannel RRKM-TST calculation. The title reaction included three manners, namely, α-C-addition, β-C-addition, and direct H-abstraction. The rate constants and branching ratios for nine product channels are calculated. It is predicted that the total rate coefficients vary with temperature, and exhibit strong positive temperature

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