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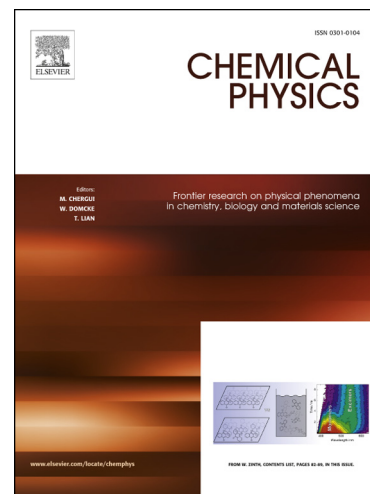
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# Mechanistic and kinetic study on the reaction of Pyrrole (C<sub>4</sub>H<sub>5</sub>N) with O(<sup>3</sup>P)

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**Abstract:** The mechanism and kinetic for the reaction of Pyrrole + O(<sup>3</sup>P) 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,  $\alpha$ -C-addition,  $\beta$ -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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