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Theoretical Study on the Initial Thermal Decomposition and Catalysis Effects of NO_2 on FOX-7

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Abstract: B3LYP/6-31G(d, p), MP4(SDTQ)/6-31G(d, p) and G3MP2B3 methods were used to calculate the energy of the decomposition species of FOX-7. Based on the energy obtained by G3MP2B3 method, the rate constants of C—NO_2 cleavage and nitro-to-nitrite rearrangement were calculated in the temperature range of 250 – 3300 K. It is found that C—NO_2 cleavage is the dominant initial thermal decomposition step at high temperature which is consistent with the conclusion based on *ab* initio molecular dynamics simulation. The effects of NO_2 on the FOX-7 decomposition were investigated. Results show that the decomposition energy barrier becomes lower when NO_2 reacts with FOX-7.

Key words: physical chemistry; thermal decomposition; FOX-7; theoretical study; rate constant; catalysis effect

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