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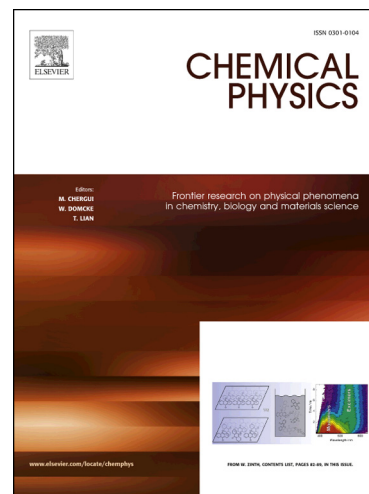
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Anharmonic Effect of the Reactions Related to Cyano Radical as Reactant in Fuel Combustion Mechanism

Rui Zhao, Duo Gao, Xinxiang Pan, Liguo Song, Hongjing Yu, Shubo Yu, Li Yao*

Dalian Maritime University, Dalian, 116026, China

*Email: yaoli@dlmu.edu.cn

Abstract: On the basis of Miller-Bowman mechanism, there are mainly eight bimolecular reactions involved in cyano radical (CN) as reactant in fuel combustion processes. In order to carry out the theoretical studies of chemical kinetics on those reactions mentioned above, all the geometries in this work have been optimized by the B3LYP method with the 6-311++G** basis set. The barrier heights have been corrected at the QCISD(T)/6-311++G** level. Using the transition state theory (TST), the anharmonic effect is also investigated by comparing the rate constants over the temperature range of 300 K to 4000 K. The kinetics and thermodynamic parameters of reaction mechanism are fitted based on the idea of the least square. Generally speaking, the rate constant increases with the temperature, and the anharmonic effect of these reactions is remarkable, especially in the high temperature environment. Our research results are close to the reference values.

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