# Rate Constant Calculations for the New Pathways of the $CN+C_2H_2$ Reaction

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CN reactions with small unsaturated hydrocarbons are very important in several gaseous media, as combustion systems, interstellar clouds, and $N_2$/hydrocarbon rich planetary atmospheres[1]. As an example of their importance in terrestrial environments is the role of the CN radical in the complex formation and destruction processes of polluting $NO_x$ species in combustion systems[2]. In this work, we have been studied of the potential energy surface for the different pathways of the reaction of $CN+C_2H_2$ (Figure1). Initial equilibrium geometries for the reactants, intermediate reactions, transition states, and product were optimized at M06L and CCSD/6-311++G** levels to all species involved in the $CN+C_2H_2=HC_3N+H$ reaction. The enthalpy value found to HCCCN pathway reaction (81.9681 kJ/mol) lies within limits of the crossed molecular beams experimental measurement (80-110 kJ/mol) at a collision energy of 21.1kJ/mol[3]. The rate constants have been calculated using transition state theory with Wigner and Eckart tunneling correction factor[4] and expressed in the Arrhenius form for temperature range of 200-4000K.

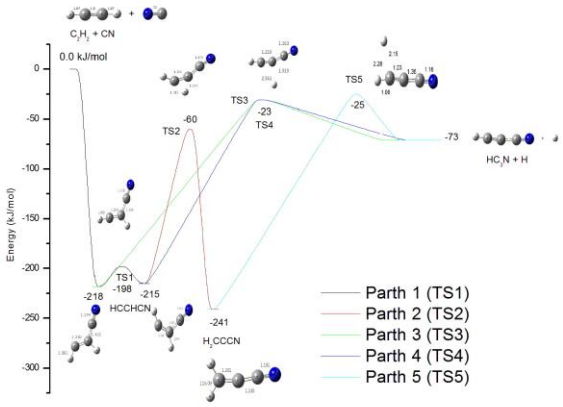


Figure1: Schematic mechanism for the $CN+C_2H_2=HC_3N+H$ reaction.

**References**

[1] N. Balucani, O. Asvany, L. C. L. Huang, Y. T. Lee, R. I. Kaiser, Y. Osamura, H. F. Bettinger, Astrophys. J., 2000, 545, 892.
[2] D. A. Lichtin, M. C. Lin, Chem. Phys. Lett., 1985, 96, 473.
[3] L. C. L. Huang, Y. T. Lee, R. I. Kaiser, J. Chem. Phys., 1999, 110, 7119.
[4] P. R .P. Barreto, A. F. A. Vilela, R. Gargano, J. of Molecular Structure (Theochem), 2003, 639, 167.