Effect of the molecular rotational energy on the N2 + H2 reactive collisions at hight translational energies

Juan de Dios Garrido Arrate [1], *Maikel Y. Ballester Furones* [2]

[1] Departmento de Física Atómica y Molecular. Instituto Superior de Tecnología y Ciencias Aplicadas, Universidad de La Habana, La Habana, Cuba
[2] Universidade Federal de Juiz de Fora, Minas Gerais, Brasil
garrido.jd@gmail.com

The shock waves created by relatively large meteorites, reentry space vehicles, and hypersonic missiles produce translational temperatures in the interval of $2000 < T/K < 45{,}000$ and higher. Under these conditions, reactions between molecular nitrogen and hydrogen are energetically permitted. In the present work a quasi-classical trajectories study of the N2 (v''=4 , 0) + H2 (v', j') reaction for relative translational energies covering the range of translational energy $30.0 \leq Etr/kcalmol(-1) \leq 130.0$ is presented. In calculations, several values of vibrational quantum numbers v' = 3, 6, 8, 10 and rotational quantum numbers j' = 2, 3, 5, 7 have been considered. To model the inter-atomic interactions, a six dimension global potential energy surface for the ground electronic state of N2H2 was used. Specific initial state reaction cross sections and rate coefficients are reported. An analysis of the possible impact of these processes on the shock wave modeling and the atmospheric composition is also presented.