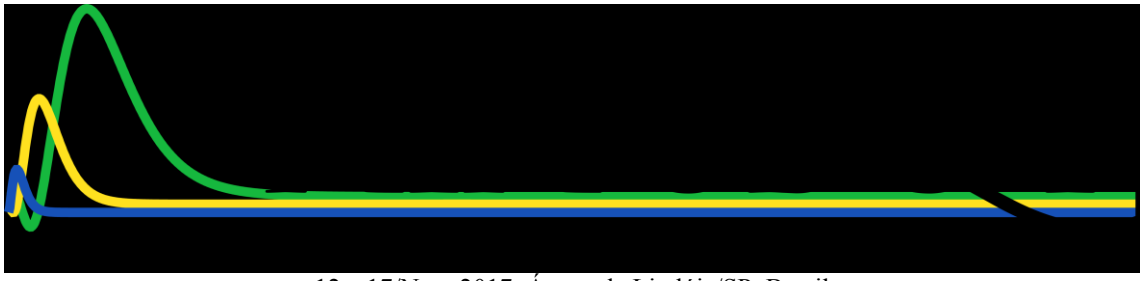

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Reactions of hypergolic pair N_2H_4 and NO_2

Marina Pelegrini[a], Marcelo A. P. Pontes[b], Luiz F. A. Ferrão[b], Orlando Roberto-Neto[c], Francisco B. C. Machado[b]

[a]*Divisão de Ensino, Academia da Força Aérea, Pirassununga – SP, Brazil,* [b]*Departamento de Química, Instituto Tecnológico de Aeronáutica, São José dos Campos-SP, Brazil,* [c]*Instituto de Estudos Avançados, Departamento de Ciências e Tecnologia Aeroespacial, São José dos Campos- SP, Brazil*

Abstract: Hydrazine (N_2H_4) and nitrogen tetroxide (N_2O_4) are well known by their energetic power especially when they are combined as a hypergolic pair, an auto ignition system. These molecules are widely utilized in aerospace applications such as rocket fuel and satellite thrusters [1]. The high reactivity of the hypergolic system was attributed to the high effectiveness of nitrogen dioxide in hydrogen abstraction of hydrazine [2]. In this work, the reactions between hydrazine and nitrogen oxide have been studied using DFT theory, with B3LYP and M062-X functionals and 6-311++G(d,p) atomic basis set. Every interaction sites have been studied and the energy diagram of the possible reactions indicates that interactions "hydrogen bond" like play crucial role in the reactions exothermicities through the intermediate species formation. The intermediate species are characterized by relative very low vibrational frequencies, indicating their low stabilities, and the higher the first frequency vibrational of the intermediate, more exothermic will be its formation. The reactants, transitions states, intermediate species and the final products N_2H_3 and HONO*cis*, HONO*trans* and HNO_2 were optimized and IRC calculations were performed to confirm the connection between reactants and intermediate species. Reactions of hydrazine with NO_2 and other molecules N-O containing had been studied by DFT calculations by Lai et al. [3,4], but the steps reaction and molecular structures are somewhat different here. In this work, two different transition states connect with an intermediate species so close in geometry with the products N_2H_3+HNO_2, by means of barrier heights around 5 and 7 kcal.mol^{-1}. Two different transition states connect with two intermediate species that are so close in geometry with the products N_2H_3+HONO*cis*, by means of barrier heights around 3 and 7 kcal.mol^{-1}. And one transition state connects with an intermediate species with barrier height like to 7 kcal.mol^{-1}. Every intermediate species are exothermic relative to reactants.

Key-words: propellant, transition state, DFT

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