XIX SBQT
Simpósio Brasileiro de Química Teórica 2017
12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

Copper Acetylacetonate Intermolecular Interactions with Conjugated Polymers

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Abstract: Hybrid propellants are of great interest in space propulsion for combining desirable characteristics of solid and liquid propulsion technologies: simplicity and operational readiness (from solid) with variable thrust and high performance (from liquid), minimizing the disadvantages associated with each one. However, a hybrid propulsion was always limited to the low rate of burning of its solid fuel, reducing its competitiveness for the transport of payload to the Earth's orbit. However, the use of paraffin has open new possibilities [1] and the application of paraffin particles agglutinated by a polymer is even more promising [2]. The latter does not exhibit excessive brittleness or melting observed in pure paraffin grains, but the high thermal degradation temperatures of the binder also reduces its propulsive performance. Thus, the improvement of the thermal degradation of the fuel is a central aspect in the development of hybrid propellants that are competitive to solid or liquid rocket engines. In this context, the present work considers adding a metal complex in the fuel to assist the thermal degradation of the polymeric binder. Specifically, a copper acetylacetonate complex ($cu(acac)_2$) was considered interacting with representative molecules of paraffin ($C_{12}H_{26}$) and fragments of hydroxyl-terminated polybutadiene ($C_{12}H_{14}$). The interaction enthalpies and free energies were computed, as well as the minimum energy paths to some dissociation channels, representing unimolecular elementary reactions which are possibly included in the thermal degradation mechanism. The stationary states and reaction paths were carried out using DFT method within M06 approximation [3] with DEF2-SVP basis set for all atoms [4]. The adsorption energies were refined by calculating the stationary states energies with CASPT2 method. The results indicate that the copper acetylacetonate complex changes the thermal degradation of the polymer acting as a catalyst and lowering the energy requirement of some dissociation channels.

Key-words: DFT, CASPT2, Hybrid Rocket, HTPB.
Support: This work has been supported by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), process Nº 309051/2016-9.

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