ENERGY AND STRUCTURAL CHARACTERISTICS FOR THE INITIAL STAGE OF SELF-IGNITION OF TRIETHYLALUMINUM IN AIR

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Abstract: The initial stages of self-ignition of triethylaluminum $Al(C_2H_5)_3$ in air are considered on the basis of the kinetic mechanism proposed by Kuznetsov *et al.* (2019). A quantum-mechanical calculation of the structures and energy characteristics of all molecular complexes involved in the processes, has been carried out. The reactions' heats were obtained and the bond energies within the complexes were found which determine the main stages of the reaction. On the basis of the energy characteristics analysis, the mechanism of triethylaluminum decomposition at the oxygen molecule intrusion is clarified. It is shown that the priority channel for the decomposition of the triethylaluminum–oxygen complex is the breaking of the bond between oxygen atoms. In this case, the total process of intrusion and decomposition is exothermic and proceeds with the release of 64.27 kJ/mol which explains the process of self-ignition.

Keywords: triethylaluminum; self-ignition; intrusion and decomposition reactions; bond energy; reaction heat; quantum mechanics

DOI: 10.30826/CE21140409

Table Captions

Table 1 Energy and geometric properties of molecules, DFT calculation, and experimental data [9]

Table 2 Geometric structures and energies of molecules participating in reactions (1)–(5)

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Received November 15, 2021

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