GAS-PHASE KINETICS OF DIBORANE OXIDATION IN AIR

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Abstract: A novel gas-phase kinetic model of diborane oxidation in air was developed. The model is based on earlier published reaction mechanisms of boron and diborane. The rate constants for some reactions were clarified in accordance with the new data obtained with the use of quantum-chemical methods. The developed mechanism including 171 reversible reactions with participation of 29 species reproduces the experimental data on the ignition of B_2H_6 with reasonable accuracy. The mechanism is used for analysing the oxidation process of diborane. The key channels of the initiation and development of the chain mechanism and products formation including the metaboric acid that significantly decreases the generation of boron oxide B_2O_3 and can lead to the heat loses during the boron-containing fuels combustion are identified.

Keywords: diborane; kinetic mechanism; ignition; modeling

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