THE CALCULATION OF THE SURFACE OF POTENTIAL ENERGY OF THE REACTION $C_5H_4O + H$ BY QUANTUM-MECHANICAL *AB INITIO* METHODS

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Abstract: The surface of potential energy of the reaction $C_5H_4O + H$ has been calculated, this reaction is the important step in the process of degradation of polycyclic and monocyclic aromatic radicals. This degradation prevents production of polycyclic aromatic hydrocarbons, which are precursors of soot in combustion systems. The geometries have been optimized with the help of the quantum chemical CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G** method. The results show that the reaction goes with the addition of hydrogen to cyclopentadienone, followed by isomerization and decomposition of carbon monoxide, giving C_4H_5 isomers. Afterwards, C_4H_5 decomposes into vinylacetylene + H and vinyl + acetylene. Rate constants and the reaction energies have been calculated.

Keywords: combustion systems; polycyclic aromatic hydrocarbons; cyclopentadienone; rate constants; potential energy surface; density functional theory; *ab initio* method

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