CALCULATION OF C–H BOND DISSOCIATION ENERGY OF 2-FURYL RADICAL AND INTERMEDIATE PRODUCTS OF ITS DECOMPOSITION USING DENSITY FUNCTIONAL THEORY AND POSSIBILITY OF HO2 FORMATION AT THE PRESENCE OF MOLECULAR OXYGEN

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Abstract: According to density functional theory (DFT) calculation, it is found that the formation of H atom by dissociation of the intermediate products of thermal decomposition of 2-furyl radical (C4H3O) is less favorable than the formation of C2H2 and CHCO, but is more likely than pathway of C3H3 and CO formation. Furthermore, the formation of HO2 due to the transfer of H atom of those products to O2 can be important when the rate of C4H3O–O2 formation does not significantly exceed the rate of thermal decomposition of the C4H3O.

Keywords: furyl radical; bio-oil; biofuel; furan; pyrolysis; molecular modeling; thermodynamics; oxidation; combustion

References


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