CALCULATION OF C–H BOND DISSOCIATION ENERGY OF 2-FURYL RADICAL AND INTERMEDIATE PRODUCTS OF ITS DECOMPOSITION USING DENSITY FUNCTIONAL THEORY AND POSSIBILITY OF HO_2 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 (C_4H_3O) is less favorable than the formation of C_2H_2 and CHCO, but is more likely than pathway of C_3H_3 and CO formation. Furthermore, the formation of HO_2 due to the transfer of H atom of those products to O_2 can be important when the rate of $C_4H_3O–O_2$ formation does not significantly exceed the rate of thermal decomposition of the C_4H_3O.

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

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Received December 18, 2015

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