STRUCTURES AND THERMOCHEMICAL PROPERTIES OF PHENOXY RADICALS FORMED FROM COMPONENTS OF THE SURROGATE BIO-OIL

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Abstract: Possible structures of radicals, produced by abstraction of the hydrogen atom from 2,4-dimethylphenol (2,4-xylenol), 2-methoxy-4-methylphenol, and 3-methoxy-4-formylphenol (vanillin), have been studied using the B3LYP/6-311++G(d,p) quantum mechanical calculations. It has been found that the phenoxy radicals are the most thermochemically stable products of these reactions. Their values of the standard enthalpies of formation as well as those values for their most important isomers are determined using thermochemistry of the isodesmotic reactions. The calculated values of the standard entropies of these radicals are also reported in the present work.

Keywords: enthalpy of formation; entropy; 2,4-dimethylphenol; 2-methoxy-4-methylphenol; 3-methoxy-4-formylphenol; phenoxy radical

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