Synthesis, Characterization, and Computational Modeling of Paeonol (2-hydroxy-4-methoxyacetophenone )

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Abstract

Paeonol (2-hydroxy-4-methoxyacetophenone) is one of the phenolic compounds that have important biological activities such as antibacterial, anti-inflammatory, allergic, and as a corrosion inhibitor. In this study, synthesis of paeonol compounds using 2,4-dihydroxyethetophenone as substrate and dimethyl formamide (DMF) as solvent. The methylation reaction is carried out using dimethyl sulfate and potassium carbonate as the catalyst. The reaction is carried out for 4 hours at room temperature. The reaction product is then extracted with aquadest mixture: ethylacetate (1: 1). The ethylacetate fraction was washed with distilled water and then separated, anhydrous Na2SO4 added, filtered and evaporated until the crude extract was obtained. The crude extract was then separated by column chromatography with eluen n-hexane: EtOAc (30: 1) to obtain a product of white powder with a melting point of 47-50 oC with a yield of 85.94%). This research could be done through computational method Hartree-Fock with SP 6-31G basis-set. The synthesis of paeonol produced the possibility of two products, these are 2-hydroxy-4-methoxyacetophenon and 2,4-dimethoxyacetophenon. Thermodynamic studies show that the 2-hydroxy-4-methoxyacetophenon and 2,4-dimethoxyacetophenon has a delta of energy -130,688 kj/mol and -112,562 kj/mol respectively, which indicates that 2-hydroxy-4-methoxyacetophenon more stable than 2,4-dimethoxyacetophenon. The result of computational studies show that synthesis paeonol produce the stable compounds in exothermic conditions.

Key Words : 2-hydroxy-4-methoxyacetophenon, 2,4-dihydroxyacetophenon, biological activities, Hartree-Fock method, exothermic.