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

Syaiful Bahri, Yuli Ambarwati, Sutopo Hadi

*Organic & Inorganic Chemistry Research Devision, Faculty of Mathematics and Natural Sciences. Universitas Lampung, Jalan S. Brojonegoro 01 Bandar Lampung, Indonesia*

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, the synthesis of paeonol compound was performed using 2,4-dihydroxyethetophenone as substrate and dimethyl formamide (DMF) as solvent. The methylation reaction was carried out using dimethyl sulfate and potassium carbonate as the catalyst. The reaction was carried out for 4 hours at room temperature. The reaction product is then extracted with mixture of H2O : ethylacetate (1 : 1). The ethylacetate fraction was washed with distilled water and then separated, added with anhydrous Na2SO4, filtered off and evaporated until the crude extract was obtained. The crude extract was then separated by column chromatography with eluents of *n*-hexane: EtOAc (30: 1) producing white powder with a melting point of 47-50 oC with a yield of 85.94%. This research could also be performed by computational method Hartree-Fock with SP 6-31G basis-set. The synthesis of paeonol produced two possibility products, i.e. 2-hydroxy-4-methoxyacetophenon and 2,4-dimethoxyacetophenon. Thermodynamic studies showed that the 2-hydroxy-4-methoxyacetophenon and 2,4-dimethoxyacetophenon have energy changes of -130,688 kj/mol and -112,562 kj/mol respectively, which indicateed that 2-hydroxy-4-methoxyacetophenon was more stable than 2,4-dimethoxyacetophenon. The result of computational studies showed that the synthesis of paeonol produced the stable compounds in exothermic conditions.

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