Solvent-Free Microwave Synthesis and DFT Characterization of Some 1,4-Diketones

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1,4-Diketones are very useful beginning molecules for the synthesis of five membered heterocycles such as pyroles, furans, thiophenes, and pyridazines\(^1\). Also, they are intermediates in synthesis of cyclopentenone derivatives\(^2\). Microwave radiation which has a synthetic importance is an alternative to conventional heating for increasing yield of the reactions. Especially solventless technique\(^3\) is clean and economic with an environmental importance\(^4\).

In this work, 1,4-diketones were synthesized via the Stetter reaction in the presence of thiazolium salt, 1,8-Diazabicyclo[5.4.0]undec-7-en, heteroaromatic carboxylic aldehydes and \(\alpha,\beta\)-unsaturated ketone under microwave irradiation. All the products were characterized by \(^1\)H NMR, \(^13\)C NMR, IR spectroscopic datas and elemental analysis. Chemical shifts of the molecules have been calculated at density functional B3LYP level. The geometries were optimized using the 6-31G(d) basis set and the following nuclear magnetic resonance calculations basis sets, respectively. The calculated NMR chemical shifts are compared with the experimental results.

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\text{R}^1: \text{2-hydroxy ethyl, R}^2: \text{Methyl, R}^3: \text{Benzyl, R}^4: \text{2-imidazolyl, 2-thiazolyl, 2-quinolyl, 3-quinolyl}
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Kaynaklar: