**ABSTRACT**

2-oxo-4-phenyl-quinoline were synthesized from ethyl benzoyl acetate. The compounds were characterized by IR, 1H NMR, 13C NMR spectra and Single-crystal X-ray diffraction studies. The theoretical studies were predicted by utilizing DFT/B3LYP and HF with 6-31G (d, p) as basis set in Gaussian 09. Natural Bond Orbital (NBO) analysis is also used to explain the molecular stability. NMR chemical shifts are calculated by using GIAO shielding tensors. The experimental results of XRD, IR, 1H NMR and 13C NMR are in very good agreement with the theoretical studies. In addition, molecular electrostatic potential (MEP) and frontier molecular orbital analysis, Fukui and local softness indices were investigated using theoretical calculations. Based on the theoretical and experimental results, the reactions conditions and the reactivity towards the electrophilic & nucleophilic attacks were predicted.